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FOOTPRINT

Functional Tools for Pesticide Risk Assessment and Management

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Deliverable DL23

Algorithms for calculation of Predicted Environmental Concentrations (PEC) based on pesticide inputs, size and discharge of water bodies

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Foreword

The present report was prepared within the context of the work package WP4 (‘Model parameterisation, meta-modelling and risk assessment) of the FOOTPRINT project (http://www.eu-footprint.org).

The preferred reference to the present document is as follows:
Reichenberger S., Bach M., Hollis J.M, Jarvis N.J., Dubus I.G., Lewis K.A., Tzilivakis J., François O. & Cerdan O. (2008). Algorithms for calculation of predicted environmental concentrations based on pesticide inputs, size and discharge of water bodies etc. Report DL23 of the FP6 EU-funded FOOTPRINT project [www.eu-footprint.org], 101 p.

Executive summary

The pesticide fate models MACRO and PRZM are used within FOOTPRINT to simulate pesticide losses from treated fields. These losses need to be converted to actual inputs into surface water and groundwater, taking into account possible risk reduction measures. Subsequently, Predicted Environmental Concentrations (PEC) have to be calculated for groundwater (PECgw) and surface water (PECsw). These concentrations can then be compared to existing legal or ecotoxicological thresholds.

In the three FOOT tools, pesticide concentrations in water resources are calculated from simulated pesticide inputs by diffuse sources (drift, surface runoff and erosion, lateral subsurface flow, and tile drainage for surface water; leaching for groundwater). In the catchment and regional scale tool FOOT-CRS, a qualitative assessment of point source inputs (e.g. farmyard runoff, accidental spills) is also offered.

For calculation of pesticide inputs into surface water within FOOT-CRS, the real surface water network is used. PECsw are calculated at the catchment outlet (i.e. for one point). In contrast, in FOOT-NES and FOOT-FS, hypothetical edge-of-field water bodies adapted from the work of FOCUS (2001) are used. PECsw and PECsed are calculated for each agro-environmental scenario, and afterwards spatially aggregated for display as map or as cumulative distribution function (CDF). PECsw are calculated separately for each input path (surface runoff + erosion + interflow; drainage; drift). In FOOT-NES and FOOT-FS, Predicted Environmental Concentrations in sediment (PECsed) and Time-Weighted Average Concentrations (TWACsw, TWACsed) are also calculated.

In FOOT-FS, the risk posed by a pesticide to the aquatic environment can be assessed by comparing predicted concentrations in surface water with aquatic ecotoxicological endpoints for the taxonomic groups used as test organisms in the registration procedure (fish, invertebrates, sediment dwelling organisms, higher aquatic plants and algae) using the data contained in the FOOTPRINT Pesticide Properties Database (PPDB). A simple toxicity/exposure ratio (TER) approach is used for this risk assessment; however, the user will be able to export the FOOTPRINT results and then perform a more sophisticated ecological risk assessment (e.g., using mesososm data or Species Sensitivity Distributions SSD) outside the FOOT tools. In FOOT-NES and FOOT-CRS, the user can obtain the (spatial or temporal, respectively) exceedance frequency of user-defined concentration thresholds from the PEC Cumulative Distribution Functions produced by the tools.

For groundwater, the same PEC calculation approach is used for FOOT-CRS and FOOT-NES. PECgw are calculated at the bottom of soil profiles and a qualitative risk assessment is performed for the deeper groundwater.

1 INTRODUCTION

The objective of Activity 4.3 of the FOOTPRINT project was to produce algorithms for calculating Predicted Environmental Concentrations (PEC) in edge-of-field surface water bodies, surface water resource abstraction points and local (shallow) groundwater. The algorithms developed or adapted within this Activity are to be included in the FOOTPRINT software tools developed in Work Package 5 (WP5). In the following, we describe the methodology used to calculate pesticide inputs into water bodies and resulting PEC for the different tools.

2 ASSESSMENT METHODOLOGY FOR DIFFUSE SOURCE INPUTS

From the MACRO and PRZM simulations, 20-year daily time series for pesticide losses (incl. the corresponding water volumes and eroded sediment yield) will be available for:

- leaching at lower boundary of the profile (MACRO)
- drainage (MACRO)
- surface runoff (infiltration excess + saturation excess runoff) (PRZM)
- erosion (PRZM)
- lateral subsurface flow (MACRO) (in practice this will also be output as drainflow)

Since the time series themselves cannot be distributed with the software due to storage issues, meaningful summary statistics (percentiles) must be derived and provided with the tools. The selected results (Table 1) from the meta-modelling exercises will then be formatted into look-up tables and stored in a MS Access database (“metamodel database”). Data will be retrieved from the database based on the relevant climate/soil/crop combination, the selected percentile, the application month, and K_{oc} and DT50 of the pesticide being modelled. The pesticide K_{oc} and DT50 parameters are by default directly taken from the FOOTPRINT PPDB. However, the user is able to override the default values with own input.

Using the results from the meta-modelling and landscape analysis (this only applies to FOOT-CRS) activities, the Predicted Environmental Concentrations (PEC) in edge-of-field surface water bodies, surface water abstraction points at the catchment outlet and groundwater are calculated. Concentrations are estimated considering potential dilution effects based on the size and discharge of the water body, water volumes associated with runoff and drainage inputs and the presence of bed sediment. In FOOT-CRS, where PECsw are to be calculated at the catchment outlet and not in edge-of-field water bodies, also geomorphological dispersion (due to different travel distances and times to the outlet) has to be taken into account.

For groundwater exposure, the main outputs will be 20-year average leachate concentration at the bottom of the profile ("PECgw") and mean annual percolation (all tools).

For surface water exposure, the main outputs will be (temporal) PECsw distributions at the catchment outlet separately for each input pathway (FOOT-CRS) or (spatial) PECsw distributions in edge-of-field water bodies separately for each input pathway (FOOT-NES). In FOOT-FS, the output will be a single PECsw value for each percentile.

One analysis (one sequence of calculation of losses, inputs and PEC) always refers to a single compound. However, the compound may be applied to more than one crop (and more than once per season) within one analysis.

<table>
<tr><th></th><th>Leaching</th><th>Drainage</th><th>Runoff</th><th>erosion</th></tr>
<tr><td>FOOT-FS</td><td rowspan="3">Extracted model output: average leaching concentration over the 20-year simulation period; flux concentrations for most soils, resident concentrations for soils with shallow groundwater, no output for soils with impermeable substrate</td><td colspan="3">(same as in FOOT-NES, since we use the same water bodies)</td></tr>
<tr><td>FOOT-CRS</td><td colspan="3">Extracted model output: maximum daily loss for each month (n = 240)</td></tr>
<tr><td>FOOT-NES</td><td colspan="3">Extracted model output: percentiles of the whole time series (return period in parentheses):
90th (10 days)
95th (20 days)
96.7th (30 days)
98.0th (50 days),
98.7th (75 days)
99.0th (100 days)
99.33th (150 days)
99.50th (200 days)
99.73th (1 year)
99.90th (about 3 years; though already very uncertain)
99.97th (about 10 years; very uncertain)
→ 11 figures
We store percentiles of the whole 20 year MACRO/PRZM time series rather than annual maxima here, because from an ecological point of view, it is more important to have information also on surface water concentrations with shorter return periods (e.g. with respect to recovery and chronic toxicity) than to have a distribution of annual maximum PECsw.</td></tr>
</table>

Table 1. Percentiles to be stored in the metamodel database

3 GROUNDWATER EXPOSURE ASSESSMENT

No percentiles of annual leaching losses or flux concentrations are stored in the Metamodel database, but the average pesticide flux concentrations over the whole simulation period of 20 years (total leaching loss over 20 years / total percolation volume over 20 years).

There are three different cases and thus meanings of pesticide leaching concentration in the metamodel database, depending on the FOOTPRINT hydrological group (cf. DL21):

a) water can percolate through lower boundary of profile → flux concentration (= total leached mass / total percolation) is calculated
b) shallow groundwater → zero flux boundary condition in MACRO → no percolation → resident concentration is calculated
c) impermeable substrate → zero flux boundary condition → no percolation → no leaching concentrations simulated (value -99 in database)

These 3 cases must be considered and treated separately in the following.

3.1 FOOT-CRS and FOOT-NES

For leaching beyond the soil profile, the PEC calculation methods are the same in FOOT-CRS and FOOT-NES.

3.1.1 PECgw calculation for a single agro-environmental scenario and a single application

The standard case is one application per year on the same area. Multiple applications per year are treated in section 3.1.2.

PECgw at the lower boundary of the soil profile are calculated as average (either flux or resident) concentrations over the whole simulation period of 20 years for the agro-environmental scenario.

$$PECgw = \{\delta MACRO(FST, Climate, Crop, Appmonth, Koc, DT50) * relDose_c\} \qquad \text{(eq. 3.1)}$$

where

PECgw	20-year average leaching flux (or resident) concentration of a.i. at the lower boundary of the soil profile for a given agro-env. scenario (unique combination of climate, NUTS-2, soil s, crop c) [$\mu g\ L^{-1}$]

δMACRO(FST, Climate, Crop, AppDate, Koc, DT50)

20-year average (flux or resident) concentration from the 20-year MACRO simulation (at bottom boundary of the soil profile) of an a.i. as a function of FOOTPRINT soil type, climate, crop, application month and compound properties [$\mu g\ L^{-1}$]

relDose,c — application rate of a.i. to crop c ($g\ ha^{-1}$) divided by the standard rate of 1000 $g\ ha^{-1}$ of the MACRO meta-model simulation

3.1.2 Dealing with multiple applications for the pathway leaching

Calculation of PECgw

The PECgw calculated in section 3.1.1 are specific for single records in the export file delivered by the Pesticide Scenario Manager. In this file, however, it is possible that a pesticide is applied within the same polygon to the same crop more than once (either in different months or even in the same month). Multiple applications to the same field cannot be treated independently of each other, though, because one field treated with one compound can only have one PECgw, and because actual concentrations would be underestimated if the additive effects of multiple applications were ignored. To avoid errors (too low PEC values, double-counting of areas) in the following aggregation procedure (sections 3.1.3 and 3.1.4), the PECgw from section 3.1.1 must be searched for multiple applications and be corrected accordingly.

At least in the first versions of FOOT-FS and FOOT_NES, multiple applications (i.e. applications on the same field in different months, for instance on winter cereals in both April and November, or even in the same month, are handled in a relatively simple way:

- The loads and thus the PECgw from the different applications are simply added up (adding up PECgw is possible because the percolation volume is always the same for the same NUTS2/climate/SMU/CLC/STU/cropID combination). This method implicitly assumes that the pesticide molecules from the different applications do not significantly interfere by changing concentration gradients between the micropore and macropore domain compared to a single application.
- However, it has additionally to be taken into account that within a polygon, the treated area fraction can differ between the different applications (cf. next section).

Procedure to enable spatial aggregation of PECgw

To make a correction of PECgw and Ftreated for multiple applications possible at all, the following important assumption is made that *application is preferential*. That is, within a crop/STU combination in a polygon there are areas that need treatment more regularly and more frequent than others. Examples:

- If in the first application 10 % of the area of the crop/STU combination are treated, and in the second application 20 % are treated, all areas treated in the first application are treated again in the second.
- If in the first application 10 % of the area of the crop/STU combination are treated, and in the second application 5 % are treated, all areas treated in the second application have also been treated in the first.

Based on this assumption, the following procedure is applied:

1. All applications with the same NUTS2/climate/SMU/CLC/STU/cropID combination are selected.

NUTS2	climate	SMU	CLC	STU	cropID	appmonth	Apprate	Ftreated	PECgw	Mean Annual Percolation
							g ha-1	(fraction)	µg L-1	mm
1	1	1	1	1	1	3	1000	0.6	0.30	100
1	1	1	1	1	1	4	500	0.5	0.10	100
1	1	1	1	1	1	4	400	0.3	0.08	100
1	1	1	1	1	1	5	600	0.2	0.05	100
1	1	1	1	1	1	5	600	0.6	0.05	100

2. All applications with the same NUTS2/climate/SMU/CLC/STU/cropID combination are sorted in descending order of Ftreated (area fraction of crop/STU combination i that is treated with the compound of concern).

NUTS2	climate	SMU	CLC	STU	crop ID	appmonth	apprate	Ftreated	PECgw	Mean Annual Percolation
							g ha-1	(fraction)	µg L-1	mm
1	1	1	1	1	1	3	1000	0.6	0.30	100
1	1	1	1	1	1	5	600	0.6	0.05	100
1	1	1	1	1	1	4	500	0.5	0.10	100
1	1	1	1	1	1	4	400	0.3	0.08	100
1	1	1	1	1	1	5	600	0.2	0.05	100

3. For all applications with the same NUTS2/climate/SMU/CLC/STU/cropID combination and the same Ftreated, PECgw are added up. The resulting record (red) is kept and the original records are deleted.

NUTS2	climate	SMU	CLC	STU	crop ID	appmonth	apprate	Ftreated	PECgw	Mean Annual Percolation
							g ha-1	(fraction)	µg L-1	mm
1	1	1	1	1	1			0.6	0.35	100
1	1	1	1	1	1	4	500	0.5	0.10	100
1	1	1	1	1	1	4	400	0.3	0.08	100
1	1	1	1	1	1	5	600	0.2	0.05	100

4. For all applications with the same NUTS2/climate/SMU/CLC/STU/cropID combination, the PECgw with the largest Ftreated (1), are added to the PECgw of the application with the next smaller Ftreated (2). (1) is then updated by subtracting (2) from it.

NUTS2	climate	SMU	CLC	STU	crop ID	appmonth	apprate	Ftreated	PECgw	Mean Annual Percolation
							g ha-1	(fraction)	µg L-1	mm
1	1	1	1	1	1			0.6 – 0.5 = 0.1	0.35	100
1	1	1	1	1	1	4	500	0.5	0.10 + 0.35 = 0.45	100
1	1	1	1	1	1	4	400	0.3	0.08	100
1	1	1	1	1	1	5	600	0.2	0.05	100

5. Repeat procedure for the next record.

NUTS2	climate	SMU	CLC	STU	crop ID	appmonth	apprate	Ftreated	PECgw	Mean Annual Percolation
							g ha-1	(fraction)	µg L-1	Mm
1	1	1	1	1	1			0.1	0.35	100
1	1	1	1	1	1	4	500	0.5 – 0.3 = 0.2	0.45	100
1	1	1	1	1	1	4	400	0.3	0.08 + 0.45 = 0.53	100
1	1	1	1	1	1	5	600	0.2	0.05	100

6. And so on, until the last record is updated.

NUTS2	climate	SMU	CLC	STU	crop ID	appmonth	apprate	Ftreated	PECgw	Mean Annual Percolation
							g ha-1	(fraction)	µg L-1	mm
1	1	1	1	1	1			0.1	0.35	100
1	1	1	1	1	1	4	500	0.2	0.45	100
1	1	1	1	1	1	4	400	0.3 – 0.2 = 0.1	0.53	100
1	1	1	1	1	1	5	600	0.2	0.05 + 0.53 = 0.58	100

7. Final table

NUTS2	climate	SMU	CLC	STU	crop ID	appmonth	apprate	Ftreated	PECgw	Mean Annual Percolation
							g ha-1	(fraction)	µg L-1	mm
1	1	1	1	1	1			0.1	0.35	100
1	1	1	1	1	1	4	500	0.2	0.45	100
1	1	1	1	1	1	4	400	0.1	0.53	100
1	1	1	1	1	1	5	600	0.2	0.58	100

The sum of Ftreated in the final table (0.60) is equal to the highest Ftreated in the starting table, which is a consequence of the preferential application assumption made above. The highest PECgw (0.58 µg L-1) in the final table (representing areas which have received all 5 applications) is equal to the sum of PECgw representing single applications in the starting table.

The final table resulting from the procedure in section 3.1.2.2 can now be used for spatial aggregation (sections 3.1.3 and 3.1.4).

3.1.3 Spatial aggregation of PECgw to map units (for map display)

There are four different options for PECgw display:

a) area-weighted mean PECgw, referring to only the treated area

b) area-weighted mean PECgw, referring to the total polygon (unique NUTS2/climate/SMU/CLC combination) area

c) flux– and area-weighted mean PECgw, referring to the total polygon area

d) maximum PEC occurring in the treated area (i.e. the highest PEC of all agro-environmental scenarios occurring in the NUTS/climate/SMU/CLC combination)

While in option c) it is implicitly assumed that groundwater is horizontally well mixed over the polygon area, in the other options it is implicitly assumed that groundwater is not well mixed horizontally.

In the spatial aggregation as area-weighted mean, two area fractions have to be considered:

I. area fraction of the NUTS2-climate-SMU-CLC combination (i.e. the polygon) that is covered by a particular STU/crop combination
II. area fraction of target crop in a NUTS2-climate-SMU-CLC combination that is treated with the pesticide of concern

Again, the area fraction covered by a particular STU/crop combination (i) is obtained as the product of the area fractions covered by the STU and by the crop of concern.

For the different output options, and separately for the different leaching concentration types (soils with leaching flux concentration and soils with resident concentration), the PECgw for each polygon (NUTS2/climate/SMU/CLC combination) is calculated as

a) area-weighted mean PECgw, referring to only the treated area:

$$\mathrm{PECgw}_{t} = \frac{\sum_{i} PECgw_i * FcropSTU_i * Ftreated_i}{\sum_{i} FcropSTU_i * Ftreated_i} \qquad \text{(eq. 3.2)}$$

where

STU	Soil Typological Unit of the SGDBE; each STU has a FST (FOOTPRINT soil type) attached to it
i	index of crop/STU combination (the summation is done over all crop/STU combinations in the polygon)
$FcropSTU_i$	area fraction of polygon covered by the crop/STU combination i
$Ftreated_i$	area fraction of crop/STU combination i that is treated with the compound of concern; this fraction only depends on the crop, not on the STU

b) area-weighted mean PEC, referring to the whole polygon area:

$$\mathrm{PECgw}_{\mathrm{p}} = PECgw_t * \frac{Atreated_{tot}}{Apolygon} \qquad \text{(eq. 3.3)}$$

where

$Atreated_{tot}$	total area in the polygon that is treated with the compound of concern and covered with STU's with the LX (leaching concentration type: flux concentration, resident concentration, no leaching) of concern
Apolygon	area of the polygon covered with STU's with the LX of concern

Combining eq. 3.2 and 3.3 yields

$$\mathrm{PECgw}_{\mathrm{p}} = \sum_i PECgw_i * FcropSTU_i * Ftreated_i \qquad \text{(eq. 3.4)}$$

c) flux- and area-weighted mean PEC, referring to the whole polygon area:

$$\mathrm{PECgw}_{\mathrm{pf}} = \frac{\sum_i PECgw_i * perc_i * FcropSTU_i * Ftreated_i}{\sum_i perc_i * FcropSTU_i} \qquad \text{(eq. 3.5)}$$

where

STU	Soil Typological Unit of the SGDBE; each STU has a FST (FOOTPRINT soil type) attached to it
i	index of crop/STU combination (the summation is done over all crop/STU combinations in the polygon)
$FcropSTU_i$	area fraction of polygon covered by the crop/STU combination i
$Ftreated_i$	area fraction of crop/STU combination i that is treated with the compound of concern; this fraction only depends on the crop, not on the STU
$perc_i$	annual percolation volume (mm) corresponding to PEC_i

The $PECgw_{pf}$ calculated with eq. 3.5 is mathematically equal to the ratio of total annual pesticide leaching load and total annual percolation volume in the polygon. It can only be calculated for soils with LX = flux concentration, since soils with LX = resident concentration have zero percolation.

In this PECgw aggregation option, the percolation volume associated with the PECgw (and thus the actual pesticide load) is considered. It is assumed here that groundwater is horizontally well mixed over the area of the polygon with LX = flux concentration. In this case, a flux- and area-weighted average (which takes into account total loads to groundwater) is more meaningful than just an area-weighted average (which would not consider that the different PECgw might result from very different loads; for instance, 0.1 $\mu g\ L^{-1}$ can result from 1 $\mu g\ m^{-2}$ pesticide load in 10 mm percolate, or from 50 $\mu g\ m^{-2}$ pesticide load in 500 mm percolate).

d) maximum PEC occurring in the treated area:

$$PECgw_m = \max(PECgw_i) \qquad \text{(eq. 3.6)}$$

3.1.4 Spatial aggregation of PECgw to user-defined areas (for display as CDF)

The methodology of CDF calculation for PECgw is identical to the methodology described for PECsw in section 4.5.5. The only difference is the pesticide variable that is to be plotted on the x-axis (PECgw instead of PECsw).

3.2 FOOT-FS

In FOOT-FS, PECgw only need to be calculated for a single agro-environmental scenario at a time. Spatial aggregation of results is therefore not necessary. PECgw for a single application are calculated the same way as in FOOT-NES and FOOT-CRS (cf. section 3.1.1). For multiple applications, PECgw from the different applications are simply added up (cf. section 3.1.2.1).

3.3 Assessment of pesticide concentrations in groundwater bodies in FOOT-CRS

Pesticide concentrations in depths greater than the bottom of the profile will be assessed only qualitatively (cf. FOOTPRINT Deliverable DL10 (Højberg et al., 2006)), using the default SUGAR map or a higher-resolved SUGAR map based on user data and a number of other user-input maps. The methodology is described in DL17 (François et al., 2007).

3.4 Assessment of pesticide concentrations in groundwater bodies in FOOT-NES

This is done qualitatively, using the default SUGAR map. The methodology is described in DL18 (Reichenberger et al., 2007) .

4 SURFACE WATER EXPOSURE ASSESSMENT

4.1 General surface water exposure scenario

4.1.1 FOOT-NES: Hypothetical surface water bodies

In comparison to FOOT-CRS (cf. section 4.1.3), the scale of the assessment is much larger for FOOT-NES (country or EU vs. catchment). Since it is not possible to perform a full-blown landscape analysis and routing of surface runoff in sufficient resolution for a whole country or even the whole of Europe, we follow a water body scenario approach in FOOT-NES. Hypothetical surface water bodies are taken and slightly adapted from the FOCUS surface water scenarios (FOCUS, 2001). In the following, the characteristics of the three surface water body types are described. For the standard case, the FOCUS dimensions for each water body type are adopted (Table 2). However, the FOOT-NES user will be able to modify the water body dimensions (except length) in the Data Manager (Module 1). All three water bodies, pond, ditch and stream, have a rectangular internal cross-section (vertical side slope).

Type of water body	Width (m)	Total length (m)	Distance from top of bank to water (m)	Minimum water depth (m)
Ditch	1	100	0.5	0.3
Stream	1	100	1.0	0.3
Pond	30	30	3.0	1

Table 2. Standard dimensions of FOOT-NES water body types (adopted from FOCUS, 2001)

Sediment properties (Table 3) are also adopted from FOCUSsw. Since the STEPS-1-2-3-4 tool (Klein, 2007a), whose equations will be used for PECsw and PECsed calculations in FOOT-NES, does not consider suspended solids, suspended solids are not included in the definition of FOOTPRINT water bodies either.

Characteristic	Value
Sediment layer depth (cm)	5
Organic carbon content (%)	5 (approx. 9% organic matter)
Dry bulk density (kg m^{-3})	800
Porosity (%)	60

Table 3. Sediment properties of all FOOT-NES and FOOT-FS water bodies (adopted from FOCUS, 2001)

The user has the possibility to make changes to the following variables:

- water body width (m)

- minimum water depth (m)
- horizontal distance from top of bank to water surface (m)
- total depth of sediment (m)
- gravimetric organic carbon content (fraction)
- sediment dry bulk density (kg dm^{-3})
- sediment porosity (dm^{-3} dm^{-3})

For all three water body types, there is a month-specific, pesticide-free baseflow, calculated as the product of the BFI (baseflow index; available for both each FST and each STU), the area-specific discharge (available as monthly means for a 30' × 30' grid (Fekete et al., 2000; the mean value is already attached to each polygon, i.e. NUTS2/climate/SMU/CLC combination) and the catchment area of each water body.

The concept of an adjacent field and an upstream catchment (Fig. 1) has in general been adopted from the FOCUS surface water scenarios. However, there are some modifications to the FOCUS concept (cf.. FOCUS, 2001) which are explained in the following:

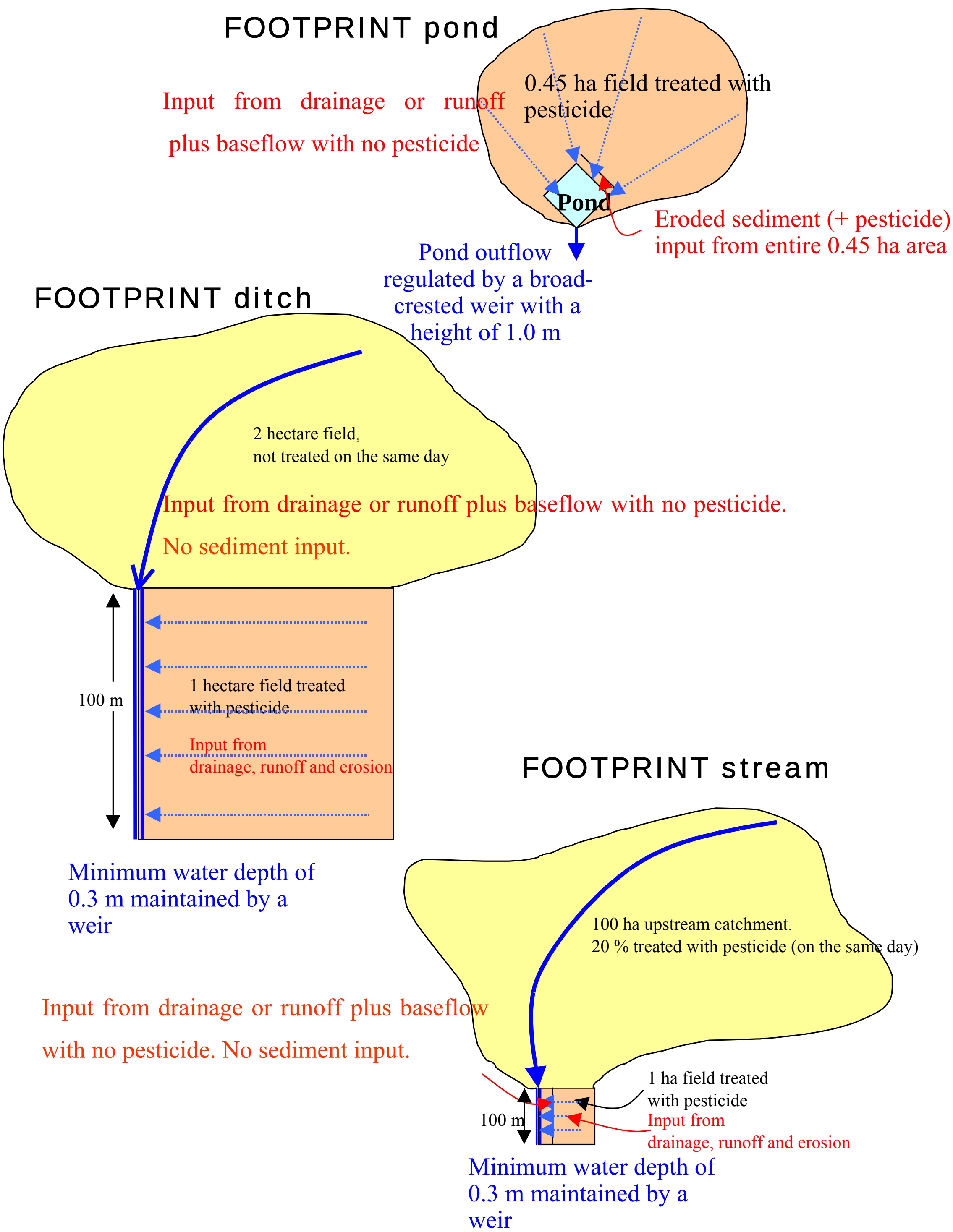

Fig. 1. Conceptual outline of the FOOT-NES and FOOT-FS water bodies (adapted from FOCUS (2001)).

- In FOOTPRINT, *all three* defined water body types (ditch, stream and pond) have an adjacent field that contributes drainage or runoff + eroded sediment (+ lateral subsurface flow, where applicable) fluxes to the water body.

- In addition, also the upstream catchment of the ditch scenario can contribute surface and subsurface runoff to the water body.
- For runoff scenarios, FOCUSsw employed a 20 m 'corridor' adjacent to the pond or stream that contributes eroded sediment and associated pesticides to the pond or stream, with the argument that eroded sediment tends to re-deposit when transported over extended distances. However, the MUSLE and MUSS equations already include deposition, because they have been obtained by regression against actual sediment loads at catchment outlets (Williams, 1975). Additionally accounting for sediment deposition is therefore conceptually wrong. *As a consequence, in FOOTPRINT the whole adjacent field contributes eroded sediment and associated pesticides to the water body.*
- While in FOCUSsw, PECsw and PECsed are calculated for simultaneous occurrences of (drift + drainflow) or (drift + runoff + erosion), in FOOT-NES and FOOT-FS PECsw are calculated separately for i) drift, ii) runoff + erosion (+lateral subsurface flow), and iii) drainflow, because we judged it not realistic that peak runoff/erosion or peak drainage inputs coincide with each other or a pesticide application day. Moreover, the influence of each input pathway on concentrations in surface waters becomes visible this way.

The following settings have been adopted from FOCUS without change:

- The fraction of the upstream catchment that is treated *on the same day* with pesticide as the adjacent field is 0 % for the ditch and 20 % of the stream. This percentage is not to be confused with the percentage of the crop that is treated at all (which is entered in the Pesticide Scenario Manager and accounted for *after* the PECsw calculation for a single scenario combination).
- No eroded soil or associated pesticide is received from the upstream catchment as all such soil is assumed to be incorporated within the upstream water body. (If the FOOT tool evaluation reveals that this yields too low estimates for erosion, this setting may be removed so that also the upstream catchment contributes eroded sediment).

In the MUSS equation, there is a slight positive correlation of area-specific sediment yield with the contributing area and a slightly negative correlation with the hydraulic length (Carsel et al., 2003). Because these effects are only slight and also counteracting, it was deemed justifiable to use the same PRZM metamodel runs (calculated for a 1 ha square field with 118.8 m hydraulic length) also for the 0.45 ha catchment of the pond.

The areas contributing pesticide inputs to the different water bodies in FOOTPRINT are summarized in Table 4.

Water Body	**Drift, drainage or runoff pesticide fluxes (dissolved) contributed from:**	**Pesticide fluxes associated with eroded sediment (adsorbed) contributed from:**
Pond	All the 0.45 ha catchment.	*All the 0.45 ha catchment*
Ditch	The adjacent 1 ha field only.	*The adjacent 1 ha field.*
Stream	The adjacent 1 ha field plus 20 ha of the upstream catchment.	*The adjacent 1 ha field.* (None from the upstream catchment)

Table 4. Areas contributing pesticide inputs (dissolved and adsorbed) to the different water bodies in FOOT-NES and FOOT-FS

It has to be noted that in FOOT-NES and FOOT-FS (as well as in FOCUSsw) it is assumed that the entire catchment of the hypothetical surface water body (adjacent field + upstream catchment) has the same soil type, the same crop type and is subject to the same weather time series.

4.1.2 FOOT-FS: Hypothetical surface water bodies

In the farm-scale tool FOOT-FS, the surface water bodies have the same upstream catchments of ditch and stream as in FOOT-NES, and the same sediment properties as the FOOT-NES default settings. However, water body dimensions (length, width, depth), size of the adjacent field (for drainage/runoff/erosion) and fraction of water body length with a field adjacent to it (for drift) are user input.

Again, the fraction of the upstream catchment that is treated *on the same day* with pesticide as the adjacent field is set to 0 % for the ditch and 20 % of the stream.

4.1.3 FOOT-CRS: Observed surface water network

In FOOT-CRS, the real (or rather, an observed) surface water network is used for calculating pesticide inputs into surface water and resulting PEC. Both the surface water network itself (as a polyline shapefile) and the catchment boundaries (as a polygon shapefile) are needed in FOOT-CRS. The default data source is the European River and Catchment Database CCM2 (Vogt et al., 2007a; Vogt et al., 2007b).

4.2 Drift inputs into surface water

4.2.1 Spray drift inputs into surface water in FOOT-NES

In FOOT-NES and FOOT-FS, PECsw are calculated for hypothetical, edge-of-field water bodies (cf. section).

Since the distance between treated field and bank of the water body is either default or user input, calculations have only to be performed for one direction.

Spray drift input for a single agro-environmental scenario and a single application

Drift input into surface water for the combination of a single agro-environmental scenario and pesticide application scenario is calculated as follows:

Lsw,drift_X = {X_drift_loading(Crop, SprayerType, Distance, Season, River Width)/1000 *absDose$_c$ *MFdrift *fAdj} (eq. 4.1)

where

Lsw,drift_X — Xth percentile area-specific daily input of an a.i. into surface waters via spray drift for a given agro-environmental scenario [mg m^{-2}]. The dimension of Lsw,drift_X is mass per surface water area, not per field area.

X_drift_loading(Crop, Application Type, Distance, Season, River Width) — estimated Xth-percentile drift loading values as a function of sprayer type (boom vs. air blast sprayer, +/- drift reducing equipment), distance edge-of-field to adjacent water body, crop stage at application (early vs. late season, only for air blast applications to pome/stone fruit), and river width [%]

(Note:

1. Distance is user input.

2. In FOOT-NES, the choice of the drift percentile is left to the user. In contrast, in FOOT-FS always the 90th percentile will be used.

3. The mathematical meaning of X_drift_loading is:

areic concentration deposited on surface water [mg m^{-2}] / application rate [mg m^{-2}] * 100 %. Hence, the application rate is also to be interpreted as an areic concentration here.

$absDose_c$	application rate (actual) of a.i. to crop c [g ha^{-1}] (user input)
MFdrift	Mitigation factor, reflecting the effects of off-field reduction measures (e.g. hedges, riparian buffers) on spray drift inputs [-]; default = 1
fAdj	fraction of the water body length that has the treated field adjacent to it [-]; in FOOT-NES, fAdj is always 1; in FOOT-FS, fAdj is user input

The variable X_drift_loading (in % of the application rate) is calculated using the drift function proposed by FOCUS (2001) and Rautmann et al. (2001). The parameters of the drift function for the different percentiles (90, 82, 77, 74, 72, 70, 69, 67, 50) have been obtained by fitting the equation to the different empirical percentiles of the BBA drift raw data (Rautmann et al., 2001).

To avoid errors in the drift calculation for those crops with a biphasic drift function, a case distinction has to be made before the drift calculation:

1. For $z_1 < H < z_2$, the integrated form of the drift equation is as follows:

$$\text{X\_drift\_loading} = \left[\frac{A}{(B+1)} * [H^{B+1} - z_1^{B+1}] + \frac{C}{(D+1)} * [z_2^{D+1} - H^{D+1}] \right] * \frac{1}{z_2 - z_1}$$

(eq. 4.2)

where

A, B, C, D = previously defined regression parameters depending on crop, sprayer type (the range of possible sprayer types in turn depends on the crop) and season

z_1 = distance from edge of treated field to closest edge of water body (m)

z_2 = distance from edge of treated field to farthest edge of water body (m)

H = distance limit for each regression (m), also called hinge point.

2. For $z_2 \leq H$, we use this formula

$$\text{X\_drift\_loading} = \frac{A}{(z_2 - z_1) * (B+1)} * [z_2^{B+1} - z_1^{B+1}] \quad \text{(eq. 4.3)}$$

3. For $z_1 \geq H$, we use this one

$$\text{X\_drift\_loading} = \frac{C}{(z_2 - z_1) * (D+1)} * [z_2^{D+1} - z_1^{D+1}] \quad \text{(eq. 4.4)}$$

In FOOT-NES, z_1 is calculated as the sum of "distance field – top of bank" from the export file created by the Pesticide Scenario Manager and "distance top of bank – water surface" (default values from FOCUS (2001) or user input). z_2 is obtained as the sum of z_1 and the water body width.

Drift mitigation measures are user input (in the Mitigation Manager, which is included in the Pesticide Scenario Manager module). Default efficiencies are provided.
Like in FOCUSsw, for the "stream" scenario drift loads Lsw,drift_X are multiplied by 1.2 to (very crudely) account for the drift input from the upstream catchment.

The pesticide drift input calculated above feeds into the PECsw calculation routines adopted from the tool STEPS-1-2-3-4 (M. Klein, IME Schmallenberg).

Dealing with multiple applications for the input pathway drift in FOOT-NES

Calculation of drift inputs

The drift inputs calculated in section 4.2.1.1 are specific for single records in the export file delivered by the Pesticide Scenario Manager. In this file, however, it is possible that a pesticide is applied within the same polygon to the same crop more than once (either in different months or even in the same month). In contrast to the soil-related pathways (runoff, erosion, drainage, leaching), for the calculation of drift inputs into surface water multiple applications to the same field can be treated independently of each other. When calculating PEC due to drift, however, multiple applications cannot be treated independently any more, because concentrations will be underestimated if at the time of application there are residues from previous application.left in the water/sediment system (cf. section 4.5.2).
Since drift inputs from different applications are independent of each other, it only has to be ensured before that there is no double-counting of areas in the following aggregation procedure (sections 4.2.1.3 and 4.2.1.4).
In FOOT-NES, drift inputs resulting from multiple applications (i.e. applications on the same field in different months, for instance on winter cereals in both April and November, or even in the same month) are dealt with as follows:

- For the spatial aggregation, the maximum drift load from the different applications is taken. This is appropriate because the aim of surface water exposure assessment is peak concentrations in water bodies, not average concentrations.
- However, it has additionally to be taken into account that within a polygon, the treated area fraction (Ftreated) can differ between the different applications.

Procedure to enable spatial aggregation of drift inputs

To make a correction of Ftreated for multiple applications possible at all, the following important assumption is made that application is preferential. That is, within the area of a given crop in a polygon there are areas that need treatment more regularly and more frequent than others. Examples:

- If in the first application 10 % of the area of the crop are treated, and in the second application 20 % are treated, all areas treated in the first application are treated again in the second.
- If in the first application 10 % of the area of the crop are treated, and in the second application 5 % are treated, all areas treated in the second application have also been treated in the first.

Based on this assumption, the following procedure is suggested:

1. All applications with the same NUTS2/climate/SMU/CLC/STU/cropID/percentile combination are selected. (Drift is independent of soil and thus STU, but the STU is part of the key identifying a record in the result table. The drift percentile is a constant within a FOOT-NES run, but to maintain consistency with the calculations for drainage/runoff/erosion, the drift percentile is used here in the key)

NUTS2	climate	SMU	CLC	STU	cropID	percentile	appmonth	Apprate	Ftreated	Drift input
								g ha-1	(fraction)	mg m-2
1	1	1	1	1	1	90	3	1000	0.6	2.0
1	1	1	1	1	1	90	4	500	0.5	1.0
1	1	1	1	1	1	90	4	400	0.3	0.8
1	1	1	1	1	1	90	5	600	0.2	4.9
1	1	1	1	1	1	90	5	600	0.6	1.0
1	1	1	1	1	1	90	6	1000	0.3	6.0
1	1	1	1	1	1	90	6	1500	0.1	7.0

2. All applications with the same NUTS2/climate/SMU/CLC/STU/cropID/percentile combination are sorted in descending order of Ftreated (area fraction of crop/STU combination i that is treated with the compound of concern).

NUTS2	climate	SMU	CLC	STU	cropID	percentile	appmonth	apprate	Ftreated	Drift input
								g ha-1	(fraction)	mg m-2
1	1	1	1	1	1	90	3	1000	0.6	2.0
1	1	1	1	1	1	90	5	600	0.6	1.0
1	1	1	1	1	1	90	4	500	0.5	1.0
1	1	1	1	1	1	90	4	400	0.3	0.8
1	1	1	1	1	1	90	6	1000	0.3	6.0
1	1	1	1	1	1	90	5	600	0.2	4.9
1	1	1	1	1	1	90	6	1500	0.1	7.0

3. For all applications with the same NUTS2/climate/SMU/CLC/STU/cropID/percentile combination and the same Ftreated, the maximum drift load is kept, and the other records are deleted.

NUTS2	Climate	SMU	CLC	STU	cropID	percentile	appmonth	apprate	Ftreated	Drift input
								g ha-1	(fraction)	mg m-2
1	1	1	1	1	1	90	3	1000	0.6	2.0
1	1	1	1	1	1	90	4	500	0.5	1.0
1	1	1	1	1	1	90	6	1000	0.3	6.0
1	1	1	1	1	1	90	5	600	0.2	4.9
1	1	1	1	1	1	90	6	1500	0.1	7.0

4. For all applications with the same NUTS2/climate/SMU/CLC/STU/cropID/percentile combination, all applications with smaller Ftreated AND smaller or equal drift load compared to the application with the largest Ftreated (here 0.6) are deleted. Applications with larger drift load remain unaffected.

NUTS2	climate	SMU	CLC	STU	cropID	percentile	appmonth	apprate	Ftreated	Drift input
								g ha-1	(fraction)	mg m-2
1	1	1	1	1	1	90	3	1000	0.6	2.0
1	1	1	1	1	1	90	4	500	0.5	1.0
1	1	1	1	1	1	90	6	1000	0.3	6.0
1	1	1	1	1	1	90	5	600	0.2	4.9
1	1	1	1	1	1	90	6	1500	0.1	7.0

NUTS2	Climate	SMU	CLC	STU	cropID	percentile	appmonth	apprate	Ftreated	Drift input
								g ha-1	(fraction)	mg m-2
1	1	1	1	1	1	90	3	1000	0.6	2.0
1	1	1	1	1	1	90	6	1000	0.3	6.0
1	1	1	1	1	1	90	5	600	0.2	4.9
1	1	1	1	1	1	90	6	1500	0.1	7.0

5. Repeat procedure for the next record (i.e. the application with the 2nd largest Ftreated).

NUTS2	Climate	SMU	CLC	STU	cropID	percentile	appmonth	apprate	Ftreated	Drift input
								g ha-1	(fraction)	mg m-2
1	1	1	1	1	1	90	3	1000	0.6	2.0
1	1	1	1	1	1	90	6	1000	0.3	6.0
1	1	1	1	1	1	90	5	600	0.2	4.9
1	1	1	1	1	1	90	6	1500	0.1	7.0

NUTS2	Climate	SMU	CLC	STU	cropID	percentile	appmonth	apprate	Ftreated	Drift input
								g ha-1	(fraction)	mg m-2
1	1	1	1	1	1	90	3	1000	0.6	2.0
1	1	1	1	1	1	90	6	1000	0.3	6.0
1	1	1	1	1	1	90	6	1500	0.1	7.0

And so on, until there is no record left which has a smaller Ftreated AND a smaller or equal drift load than another record.

6. Finally, update each Ftreated by subtracting the next smaller Ftreated from it.

NUTS2	Climate	SMU	CLC	STU	cropID	percentile	appmonth	apprate	Ftreated	Drift input
								g ha-1	(fraction)	mg m-2
1	1	1	1	1	1	90	3	1000	0.6 – 0.3 = 0.3	2.0
1	1	1	1	1	1	90	6	1000	0.3 – 0.1 = 0.2	6.0
1	1	1	1	1	1	90	6	1500	0.1	7.0

7. Final table

NUTS2	Climate	SMU	CLC	STU	cropID	percentile	appmonth	apprate	Ftreated	Drift input
								g ha-1	(fraction)	mg m-2
1	1	1	1	1	1	90	3	1000	0.3	2.0
1	1	1	1	1	1	90	6	1000	0.2	6.0
1	1	1	1	1	1	90	6	1500	0.1	7.0

The sum of Ftreated in the final table (0.60) is equal to the highest Ftreated in the starting table, which is a consequence of the preferential application assumption made above. The interpretation of the final table is: 30 % of the crop area have caused a maximum drift input of 2.0 mg m^{-2} into surface water, 20 % have caused a maximum drift input of 6.0 mg m^{-2}, and 10 % a max. drift input of 7.0 mg m^{-2}.

The final drift input table resulting from the procedure in section 4.2.1.2.2 can now be used for spatial aggregation (sections 4.2.1.3 and 4.2.1.4). The drift input maps and CDF’s will show maximum daily drift inputs into surface water from a given area over a year, NOT monthly sums of drift input.

Spatial aggregation of drift inputs to map units in FOOT-NES (for map display)

In contrast to FOOT-CRS, in FOOT-NES the agro-environmental scenario shapefile undergoes a “dissolve” operation in the Data + Scenario Manager (Module 1) with the variables NUTS2, climate, SMU and CLC class. As a consequence, each combination of NUTS2/climate/SMU/CLC in the shapefile is unique and corresponds to exactly one polygon. For losses, inputs and PEC, the treated area fraction is accounted for during the spatial aggregation in FOOT-NES.

Results from all the different relevant (i.e. with application of the pesticide of concern) agro-environmental scenarios (NUTS2-climate-soil-crop combinations) represent the range of drift inputs resulting from relevant spatial variability in the area of interest. However, for map display on polygon basis, the drift inputs have to be aggregated to only one value per polygon.

Furthermore, the user has to specify in the output options of the FOOT-NES modelling module in which format he/she wants the drift input for a polygon to be displayed:

a) area-weighted mean drift input, referring to only the treated area
b) area-weighted mean drift input, referring to the total polygon (unique NUTS2/climate/SMU/CLC combination) area

c) maximum drift input occurring in the treated area (i.e. the highest drift input of all agro-environmental scenarios occurring in the NUTS/climate/SMU/CLC combination)

All three options have meaningful interpretations. However, option a) can yield much higher values than option b).

In the spatial aggregation as area-weighted mean, two area fractions have to be considered:
I. area fraction of the NUTS2-climate-SMU-CLC combination (i.e. the polygon) that is covered by a particular crop
II. area fraction of target crop in a NUTS2-climate-SMU-CLC combination that is treated with the pesticide of concern ("fraction treated")

For the different output options, the area-specific drift input for the polygon is calculated as

a) area-weighted mean drift input, referring to only the treated area:

$$\mathrm{Lsw, drift\_X_t} = \frac{\sum_i \mathrm{Lsw, drift\_X}_i * Fcrop_i * Ftreated_i}{\sum_i Fcrop_i * Ftreated_i} \qquad \text{(eq. 4.5)}$$

where

i	index of FOOTPRINT crop (the summation is done over all FOOTPRINT crops in the polygon)
$Fcrop_i$	area fraction of polygon covered by crop i
$Ftreated_i$	area fraction of crop i that is treated with the compound of concern

b) area-weighted mean PEC, referring to the whole polygon area:

$$\mathrm{Lsw, drift\_X_p} = \mathrm{Lsw, drift\_X}_t * \frac{Atreated_{tot}}{Apolygon} \qquad \text{(eq. 4.6)}$$

where

$Atreated_{tot}$	total area in the polygon that is treated with the compound of concern
Apolygon	area of the polygon

Combining eq. 4.5 and 4.6 yields

$$\text{Lsw,drift\_X}_\text{p} = \sum_i \text{Lsw,drift\_X}_i * Fcrop_i * Ftreated_i \qquad \text{(eq. 4.7)}$$

c) maximum area-specific drift input occurring in the treated area:

$$\text{Lsw,drift\_X}_\text{m} = \max(\text{Lsw,drift\_X}_\text{i}) \qquad \text{(eq. 4.8)}$$

Spatial aggregation of drift inputs to user-defined areas in FOOT-NES (for display as CDF)

The methodology of CDF calculation for drift inputs into surface water is identical to the methodology described for PECsw in section 4.5.5. The only difference is the pesticide variable to be plotted on the x-axis.

4.2.2 Spray drift inputs in FOOT-FS

In FOOT-FS, spray drift inputs only need to be calculated for a single agro-environmental scenario at a time. Spatial aggregation of results is therefore not necessary. Spray drift inputs for a single application are calculated the same way as in FOOT-NES (cf. section 4.2.1). Multiple applications do not affect drift inputs per event, but calculation of PECsw/sed (cf. section 4.5.2).

4.2.3 Spray drift inputs in FOOT-CRS

In FOOT-CRS, drift inputs are calculated on a grid basis.

Spray drift inputs for a single map unit, crop and single application

1st step: For 8 possible wind directions (N, NE, E, SE, S, SW, W, NW), the total drift input from one map unit (one 5 × 5 m^2 pixel), one crop and one direction into surface water bodies in the catchment is calculated with the following formula:

$\text{Lsw,drift,dir\_X}_{r,c}$ = {X_drift_loading(SprayerType, Distance, Season, River Width)/1000 *$\text{absDose}_{r,c}$ *$\text{Fcrop}_{r,c}$ *$\text{Ftreated}_{r,c}$ *MFdrift_r}

where

Lsw,drift,dir_X	X^{th} percentile daily input of an a.i. into surface waters via spray drift in the area of interest, for a given wind direction [mg m^{-2}]. The dimension of Lsw,drift,dir_X is mass per surface water area, not per field area!

X_drift_loading(SprayerType, Distance, Season, River Width)

estimated X^{th}-percentile drift loading values as a function of sprayer type (boom vs. air blast sprayer, +/- drift reducing equipment), distance edge-of-field to adjacent water body, crop stage at application (early vs. late season, only for air blast applications to pome/stone fruit), and river width [%]

(Note:

1. The distance to the nearest water body in the direction of concern is calculated in the GIS, using the observed surface water network
2. The user is able to specify (legal) minimum spraying distances.
3. The 90^{th} drift percentile is suggested as default value. However, the final choice of the percentile is left to the FOOT-CRS user.
4. The mathematical meaning of X_drift_loading is:

areic concentration deposited on surface water [mg m^{-2}] / application rate [mg m^{-2}] * 100 %. Hence, the application rate is also to be interpreted as an areic concentration here.

$absDose_{r,c}$	application rate (actual) of a.i. to crop *c* in map unit *r* [g ha^{-1}] (user input)
$Fcrop_{r,c}$	area fraction of map unit *r* that is cropped with field crop *c* [-]. Given the small size of the pixels (25 m^2) compared to agricultural fields, an $Fcrop_{r,c}$ of e.g. 0.5 for winter wheat does not really mean that 50 % of the pixel are cropped with winter wheat, but rather that the probability of the pixel being cropped with winter wheat is 50 %.
$Ftreated_{r,c}$	area fraction of crop *c* in map unit r treated with the a.i. (reflects plant protection intensity and "market share") [-] (user input in the Pesticide Scenario Manager)
$MFdrift_r$	Mitigation factor, reflecting the effects of off-field reduction measures (e.g. hedges, riparian buffers) for spray drift inputs from map unit *r* [-]. In FOOT-CRS, $MFdrift_r$ is explicitly calculated in the GIS using the landscape feature map provided by the user (cf. DL17).

r	Map unit index (in FOOT-CRS, map units for drift calculation are pixels; the input into the catchment is calculated by summing up over all pixels in the catchment.)
c	Crop index

The variable X_drift_loading (in % of the application rate) is calculated using the drift function proposed by FOCUS (2001) and Rautmann et al. (2001). The parameters of the drift function for the different percentiles (90, 82, 77, 74, 72, 70, 69, 67, 50) have been obtained by fitting the equation to the different empirical percentiles of the BBA drift raw data (Rautmann et al., 2001).

To avoid errors in the drift calculation for those crops with a biphasic drift function, a case distinction has to be made before the drift calculation:

1. For $z_1 < H < z_2$, the integrated form of the drift equation is as follows:

$$\text{X\_drift\_loading} = \left[\frac{A}{(B+1)} * [H^{B+1} - z_1^{B+1}] + \frac{C}{(D+1)} * [z_2^{D+1} - H^{D+1}] \right] * \frac{1}{z_2 - z_1}$$

(eq. 4.9)

where

A, B, C, D = previously defined regression parameters depending on crop, sprayer type (the range of possible sprayer types in turn depends on the crop) and season

z_1 = distance from edge of treated field to closest edge of water body (m). z_1 is calculated as z - river_width/2).

z_2 = distance from edge of treated field to farthest edge of water body (m). z_2 is calculated as z + river_width/2).

H = distance limit for each regression (m), also called hinge point.

z = Distance from the agricultural map unit (pixel) to the water body (polyline segment); directly calculated in the GIS.

river_width = water body width; obtained from combining the UNH-GRDC dicharge map with a width-discharge relation derived by Pistocchi and Pennington (2006).

2. For $z_2 \leq H$, we use this formula:

$$\text{X\_drift\_loading} = \frac{A}{(z_2 - z_1) * (B+1)} * [z_2^{B+1} - z_1^{B+1}] \quad \text{(eq. 4.10)}$$

3. For $z_1 \geq H$, we use this one:

$$X\_drift\_loading = \frac{C}{(z_2 - z_1) * (D+1)} * [z_2^{D+1} - z_1^{D+1}] \qquad \text{(eq. 4.11)}$$

2nd step: The drift inputs into the catchment for the different wind directions (Lsw,drift,dir_X) are averaged using the unweighted or a weighted (with the probabilities of occurrence of the different wind directions) arithmetic mean. The weighting has to be done by the user. The resulting variable is called Lsw,drift_$X_{r,c}$.

Create maps of drift inputs

In contrast to FOOT-NES, in FOOT-CRS

- Pixels (as opposed to polygons) are the basis for drift map display.
- The „Fraction treated“ is already contained in the input calculations and thus doesn't need to be considered here any more.
- Drift input maps (expressed as inputs FROM each agricultural pixel into sw; "type I") are created for each application date. The total drift input into surface water (again per m^2 surface water area) from each pixel at a given application date is obtained as:

  $$\text{Lsw,drift\_X}_r = \sum_c \text{Lsw,drift\_X}_{r,c} \qquad \text{(eq. 4.12)}$$

with

r	Map unit index (in FOOT-CRS, map units for drift calculation are pixels; the input into the catchment is calculated by summing up over all pixels in the catchment.)
c	Crop index

- Drift input maps (expressed as inputs INTO each surface water pixel; "type II") are created for each application date

The drift input grids can be displayed as is. An aggregation of these grids to the polygons of the agro-environmental scenario map is not possible.

Since the drift input calculated using the Ganzelmeier/Rautmann tables refers to m^2 surface water area, NOT to m^2 field area, it is NOT possible to obtain total drift input into the catchment (cf. section 4.2.3.5) by just summing up over the pixels of the type I grids. For this reason, the type II grids must be created. With the grid map of drift inputs into surface water pixels one can easily aggregate drift inputs over the catchment by summing up over all surface water pixels.

Spatial aggregation of drift inputs to user-defined areas in FOOT-CRS (for display as CDF)

In one FOOT-CRS run, several cumulative distribution functions (CDF) of drift inputs are produced (one for each application date).

Because each pixel has the same area and the treated area fraction has already been considered beforehand, the methodology of CDF calculation for drift inputs into surface water is much simpler than the methodology described for PECsw in section 9.4. The CDF of pesticide drift inputs FROM agricultural areas (in mg per m2 surface water area) can be obtained by simply ranking the pixels in ascending order of drift input and calculating the cumulative relative frequency with

cumulative rel. frequency of a pixel = rank of pixel / total number of pixels * 100 %. (eq. 4.13)

In one FOOT-CRS run, several cumulative distribution functions (CDF) of drift inputs are produced (one for each application date).

Summing up drift inputs over the catchment area for PECsw calculation

For each application date, the daily drift inputs INTO a surface water pixel (calculated in section 4.2.3.3) are summed up over the catchment area → $Lsw,drift\_X_{catch}$ (mg).

4.3 Drainage inputs into surface water

4.3.1 Drainage inputs in FOOT-NES

There are three different cases and thus meanings of pesticide drainage losses in the metamodel database, depending on the FOOTPRINT hydrological group (cf. DL21):

a) soil is artificially drained → variables in the MM database denote actual pesticide drainage loss and corresponding drainflow volume

b) soil is not artificially drained, but lateral subsurface flow (interflow) occurs → variables in the MM database denote pesticide loss via subsurface flow and corresponding interflow volume

c) soil is neither artificially drained nor does interflow occur → no drainage loss simulated (value -99 in database)

These 3 cases must be considered and treated separately in the following.

Drainage losses and inputs for a single agro-environmental scenario and a single application

Pesticide drainage input into surface water for the combination of a single agro-environmental scenario and pesticide application scenario is calculated as follows:

Lsw,drain_X = {X_drainloss_MACRO(FST, Climate, Crop, Appmonth, Koc, DT50) *relDose$_c$ * MFdrain} (eq. 4.14)

where

Lsw,drain_X	Xth percentile daily input of a.i. into surface waters via tile drains for a given agro-env. scenario (unique combination of climate, NUTS-2, soil s, crop c) [mg m^{-2}]
X_drainloss_MACRO(FST, Climate, Crop, AppDate, Koc, DT50)	Xth-percentile (of the 20-year simulation period) daily pesticide drainage loss of a.i. as a function of soil type, climate, crop, application month and compound properties [mg m^{-2}]
relDose$_c$	application rate of a.i. to crop *c*, relative to the standard rate of 1000 g ha^{-1} of the MACRO meta-model simulation [-]
MFdrain	Mitigation factor, reflecting the effects of reduction measures on pesticide drainage inputs into surface water; default = 1

The pesticide drainage input calculated above feeds into the PECsw calculation routines adopted from the tool STEPS-1-2-3-4 (M. Klein, IME Schmallenberg).

Dealing with multiple applications for the input pathway drainage

Calculation of drainage losses and inputs

The drainage inputs calculated in section 4.3.1.1 are specific for single records in the export file delivered by the Pesticide Scenario Manager. In this file, however, it is possible that a pesticide is applied within the same polygon to the same crop more than once (either in different months or even in the same month). In contrast to drift, for the calculation of drainage (as well as runoff and erosion) inputs into surface water multiple applications to the same field cannot be treated independently of each other, since residues from one application might still be present in the field at the time of the next application. Additionally, it has to be ensured that there is no double-counting of areas in the following aggregation procedure (sections 4.3.1.3 and 4.3.1.4).

In contrast to drift, for the pathways runoff, erosion and drainage input events are triggered by rainfall events, not by pesticide application. If two applications take place in the same calendar month, it can be assumed that the pesticide runoff/erosion or drainage inputs from the two applications occur on the same day. So there is no carryover in water and sediment (because there is only one input event), but there is some carryover in the field from the first application to the second.

In FOOT-NES, pesticide drainage inputs resulting from multiple applications (i.e. applications on the same field in different months, for instance on winter cereals in both April and November, or even in the same month) are dealt with as follows:

- If there are two or more applications in different calendar months, they are treated as independent.
- If there are two more applications in the same calendar month, we update the pesticide application rates by calculating the residues from the first application in the field and adding them to the application rate of the second application (the process is repeated for additional applications). In mathematical form:

Be there n applications, application_1 at t_1, application_2 at t_2, application_n at t_n.

For a single application, the residues from that application at time t are obtained as:

residue (t) = application_rate * exp (- ln2/DT50 * t) (eq. 4.15)

For a sequence of applications, it follows:

application_rate_2_updated = application_rate_1 * exp (- ln2/DT50 * (t_2 - t_1)) + application_rate_2 (eq. 4.16)

application_rate_3_updated = application_rate_2_updated * exp (- ln2/DT50 * (t_2 - t_1)) + application_rate_3 (eq. 4.17)

application_rate_n_updated = application_rate_n-1_updated * exp (- ln2/DT50 * (t_n – t_{n-1})) + application_rate_n. (eq. 4.18)

- Then ALL updated application rates (application rate + residues from previous applications) within each calendar month are used together with the metamodel output to calculate drainage losses and inputs (cf. section 4.3.1.1).
- Subsequently, ALL resulting pesticide inputs into sw within each calendar month are used to run STEPS (cf. section 4.5.1).

- For the spatial aggregation, the maximum drainage loss/input from the different application is taken. This is appropriate because the aim of surface water exposure assessment is peak concentrations in water bodies, not average concentrations.
- However, it has additionally to be taken into account that within a polygon, the treated area fraction (Ftreated) can differ between the different applications.

Procedure to enable spatial aggregation of drainage losses and inputs

To make a correction of Ftreated for multiple applications possible at all, the following important assumption is made that application is preferential. That is, within the area of a given crop in a polygon there are areas that need treatment more regularly and more frequent than others. Examples:

- If in the first application 10 % of the area of the crop are treated, and in the second application 20 % are treated, all areas treated in the first application are treated again in the second.
- If in the first application 10 % of the area of the crop are treated, and in the second application 5 % are treated, all areas treated in the second application have also been treated in the first.

Based on this assumption, the following procedure is suggested. The procedure has to be performed for both pesticide drainage losses and inputs (the updated values from section 4.3.1.2.1).

1) All applications with the same NUTS2/climate/SMU/CLC/STU/cropID/percentile combination are selected. To keep the complexity of the calculations at a manageable level, the calculations are performed as if the previous applications that contributed to the updated application rates and thus to pesticide drainage losses/inputs of a particular record had the same treated area fractions as the application listed in the record (which is usually not correct, of course).

NUTS2	climate	SMU	CLC	STU	cropID	per-centile	appmonth	Application rate (updated)	Ftreated	Daily pesticide drainage loss/input (updated)
								g ha-1	(fraction)	mg m-2
1	1	1	1	1	1	95	4	1000	0.6	2.0
1	1	1	1	1	1	95	4	500	0.6	1.0
1	1	1	1	1	1	95	4	400	0.3	0.8
1	1	1	1	1	1	95	5	600	0.2	4.9
1	1	1	1	1	1	95	5	600	0.6	1.0
1	1	1	1	1	1	95	6	1000	0.3	6.0
1	1	1	1	1	1	95	6	1500	0.1	7.0

2) All applications with the same NUTS2/climate/SMU/CLC/STU/cropID/percentile combination are sorted in descending order of Ftreated (area fraction of crop/STU combination i that is treated with the compound of concern).

NUTS2	climate	SMU	CLC	STU	cropID	per-centile	appmonth	Application rate (updated)	Ftreated	Daily pesticide drainage loss/input (updated)
								g ha-1	(fraction)	mg m-2
1	1	1	1	1	1	95	4	1000	0.6	2.0
1	1	1	1	1	1	95	4	500	0.6	1.0
1	1	1	1	1	1	95	5	600	0.6	1.0
1	1	1	1	1	1	95	4	400	0.3	0.8
1	1	1	1	1	1	95	6	1000	0.3	6.0
1	1	1	1	1	1	95	5	600	0.2	4.9
1	1	1	1	1	1	95	6	1500	0.1	7.0

3) For all applications with the same NUTS2/climate/SMU/CLC/STU/cropID/percentile combination and the same Ftreated, the maximum drainage loss/input is taken, and the other records are deleted.

NUTS2	Climate	SMU	CLC	STU	cropID	per-centile	appmonth	Application rate (updated)	Ftreated	Daily pesticide drainage loss/input (updated)
								g ha-1	(fraction)	mg m-2
1	1	1	1	1	1	95	4	1000	0.6	2.0
1	1	1	1	1	1	95	6	1000	0.3	6.0
1	1	1	1	1	1	95	5	600	0.2	4.9
1	1	1	1	1	1	95	6	1500	0.1	7.0

4) For all applications with the same NUTS2/climate/SMU/CLC/STU/cropID/percentile combination, ALL applications with smaller Ftreated AND smaller or equal drainage loss/input compared to the application with the largest Ftreated (here 0.6) are deleted. Applications with larger drainage loss/input remain unaffected.

NUTS2	Climate	SMU	CLC	STU	cropID	per-centile	appmonth	Application rate (updated)	Ftreated	Daily pesticide drainage loss/input (updated)
								g ha-1	(fraction)	mg m-2
1	1	1	1	1	1	95	4	1000	0.6	2.0
1	1	1	1	1	1	95	6	1000	0.3	6.0
1	1	1	1	1	1	95	5	600	0.2	4.9
1	1	1	1	1	1	95	6	1500	0.1	7.0

5) Repeat procedure for the next record (i.e. the application with the 2nd largest Ftreated).

NUTS2	Climate	SMU	CLC	STU	cropID	per-centile	appmonth	Application rate (updated)	Ftreated	Daily pesticide drainage loss/input (updated)
								g ha-1	(fraction)	mg m-2
1	1	1	1	1	1	95	4	1000	0.6	2.0
1	1	1	1	1	1	95	6	1000	0.3	6.0
1	1	1	1	1	1	95	5	600	0.2	4.9
1	1	1	1	1	1	95	6	1500	0.1	7.0

NUTS2	Climate	SMU	CLC	STU	cropID	per-centile	appmonth	Application rate (updated)	Ftreated	Daily pesticide drainage loss/input (updated)
								g ha-1	(fraction)	mg m-2
1	1	1	1	1	1	95	4	1000	0.6	2.0
1	1	1	1	1	1	95	6	1000	0.3	6.0
1	1	1	1	1	1	95	6	1500	0.1	7.0

And so on, until there is no record left which has a smaller Ftreated AND a smaller or equal drainage loss/input than another record.

6) Finally, update each Ftreated by subtracting the next smaller Ftreated from it.

NUTS2	Climate	SMU	CLC	STU	cropID	per-centile	appmonth	Application rate (updated)	Ftreated	Daily pesticide drainage loss/input (updated)
								g ha-1	(fraction)	mg m-2
1	1	1	1	1	1	95	4	1000	0.6 – 0.3 = 0.3	2.0
1	1	1	1	1	1	95	6	1000	0.3 – 0.1 = 0.2	6.0
1	1	1	1	1	1	95	6	1500	0.1	7.0

7) Final table

NUTS2	Climate	SMU	CLC	STU	cropID	per-centile	appmonth	Application rate (updated)	Ftreated	Daily pesticide drainage loss/input (updated)
								g ha-1	(fraction)	mg m-2
1	1	1	1	1	1	95	4	1000	0.3	2.0
1	1	1	1	1	1	95	6	1000	0.2	6.0
1	1	1	1	1	1	95	6	1500	0.1	7.0

The sum of Ftreated in the final table (0.60) is equal to the highest Ftreated in the starting table, which is a consequence of the preferential application assumption made above. The interpretation of the final table is: 30 % of the crop area have caused a maximum daily drainage loss/input of 2.0 mg m^{-2} into surface water, 20 % have caused a maximum daily drainage loss/input of 6.0 mg m^{-2}, and 10 % a maximum daily drainage loss/input of 7.0 mg m^{-2}.

The final drainage loss/input resulting from the procedure in section 4.3.1.2 can now be used for spatial aggregation (sections 4.3.1.3 and 4.3.1.4).

Spatial aggregation of drainage inputs to map units in FOOT-NES (for map display)

In contrast to FOOT-CRS, in FOOT-NES the scenario shapefile undergoes a "dissolve" operation in the Scenario Manager (Module 2) with the variables NUTS2, climate, SMU and CLC class. As a consequence, each combination of NUTS2/climate/SMU/CLC is unique and corresponds to exactly one polygon.

For losses, inputs and PEC, the treated area fraction is accounted for during the spatial aggregation in FOOT-NES.
Results from all the different relevant (i.e. with application of the pesticide of concern) agro-environmental scenarios (NUTS2/climate/soil/crop combinations) represent the range of drainage inputs resulting from relevant spatial variability in the area of interest. However, for map display on polygon basis, the drainage inputs have to be aggregated to only one value per polygon.

Furthermore, the user has to specify in the output options of the FOOT-NES modelling module in which format he/she wants the drainage inputs for a polygon to be displayed:

a) area-weighted mean drainage input, referring to only the treated area
b) area-weighted mean drainage input, referring to the total polygon (unique NUTS2/climate/SMU/CLC combination) area
c) maximum drainage input occurring in the treated area (i.e. the highest drainage input of all agro-environmental scenarios occurring in the NUTS/climate/SMU/CLC combination)

All three options have meaningful interpretations. However, option a) can yield much higher values than option b).

In the spatial aggregation as area-weighted mean, two area fractions have to be considered:
I. area fraction of the NUTS2-climate-SMU-CLC combination (i.e. the polygon) that is covered by a particular STU/crop combination
II. area fraction of target crop in a NUTS2-climate-SMU-CLC combination that is treated with the pesticide of concern

In reality, crops and soil types are to some degree statistically dependent (for instance, potatoes are usually not grown on heavy clays). However, given the number of FOOTPRINT crops and soil types and the fact that the dependence of the occurrence of a given crop on the soil type probably varies with climate, it is impossible to estimate crop/soil dependencies on a European level. It is therefore justifiable to assume that FOOTPRINT crops and soil types are statistically independent. Consequently, the area fraction covered by a particular STU/crop combination (i) is obtained as the product of the area fractions covered by the STU and by the crop of concern.

For the different output options, and separately for the different percentiles and drainage types (actual drainflow vs. lateral subsurface flow), the area-specific drainage input for the polygon is calculated as

a) area-weighted mean drainage input, referring to only the treated area:

$$\mathrm{Lsw,drain\_X_t} = \frac{\sum_i \mathrm{Lsw,drain\_X}_i * FcropSTU_i * Ftreated_i}{\sum_i FcropSTU_i * Ftreated_i} \qquad \text{(eq. 4.19)}$$

where

STU	Soil Typological Unit of the SGDBE; each STU has a FST (FOOTPRINT soil type) attached to it
i	index of crop/STU combination (the summation is done over all crop/STU combinations in the polygon)
$FcropSTU_i$	area fraction of polygon covered by the crop/STU combination i
$Ftreated_i$	area fraction of crop/STU combination i that is treated with the compound of concern; this fraction only depends on the crop, not on the STU

b) area-weighted mean drainage input, referring to the whole polygon area:

$$\mathrm{Lsw,drain\_X_p} = \mathrm{Lsw,drain\_X}_t * \frac{Atreated_{tot}}{Apolygon} \qquad \text{(eq. 4.20)}$$

where

$Atreated_{tot}$	total area in the polygon that is treated with the compound of concern and covered with STU's with the drainflow type of concern (actual drainflow or lateral subsurface flow)
Apolygon	area of the polygon covered with STU's with the drainflow type of concern (actual drainflow or lateral subsurface flow)

Combining eq. 4.19 and 4.20 yields

$$\mathrm{Lsw,drain\_X_p} = \sum_i \mathrm{Lsw,drain\_X}_i * FcropSTU_i * Ftreated_i \qquad \text{(eq. 4.21)}$$

c) maximum drainage input occurring in the treated area:

$$Lsw,drain\_X_m = \max (Lsw,drain\_X_i) \qquad \text{(eq. 4.22)}$$

The described aggregation methodology for pesticide inputs into surface water also applies to pesticide drainage losses, of course.

Spatial aggregation of drainage inputs to user-defined ares in FOOT-NES (for display as CDF)

The methodology of CDF calculation for drainage inputs into surface water (or drainage losses) is identical to the methodology described for PECsw in section 4.5.5. The only difference is the pesticide variable to be plotted on the x-axis.

4.3.2 Drainage inputs in FOOT-FS

In FOOT-FS, drainage inputs only need to be calculated for a single agro-environmental scenario at a time. Spatial aggregation of results is therefore not necessary. Drainage inputs for a single application are calculated the same way as in FOOT-NES (cf. section 4.3.1.1).
Like in FOOT-NES, multiple applications are considered by updating the application rates with the residues present in the field from previous applications (cf. section 4.3.1.2.1). However, in contrast to FOOT-NES, where applications in different calendar months are treated as independent, in FOOT-FS residues from applications in one calendar month are carried over to applications of the same active in the next month (provided the interval between the last application in one calendar month and the first application in the following month is not longer than 28 days).
Subsequently, the highest updated application rate (application rate + residues from previous applications) within each calendar month is selected and used together with the metamodel output to calculate drainage losses and inputs (cf. section 4.3.1.1) and to run STEPS (cf. section 4.5.1)

4.3.3 Drainage inputs in FOOT-CRS

In contrast to drift and runoff/erosion, no grid calculations are necessary to calculate drainage inputs into surface water in FOOT-CRS. The approach is therefore almost identical to the approach in FOOT-NES.

In contrast to FOOT-NES and FOOT-FS, the FOOT-CRS metamodel database does not contain 11 pesticide loss percentiles of the whole 20-year time series, but monthly maxima of pesticide loss for each month, i.e. 240 values for each simulation run (cf. chapter 2).

Drainage losses and inputs for a single agro-environmental scenario and a single application

Pesticide drainage input into surface water for the combination of a single agro-environmental scenario and pesticide application scenario is calculated as follows:

Lsw,drain_m = {m_drainloss_MACRO(FST, Climate, Crop, Appmonth, Koc, DT50) *$relDose_c$ * MFdrain} (eq. 4.23)

where

Lsw,drain_m	maximum daily input of a.i. into surface waters via tile drains in month m (m = 1-240) for a given agro-env. scenario (unique combination of climate, NUTS-2, soil s, crop c) [mg m^{-2}]
m_drainloss_MACRO(FST, Climate, Crop, AppDate, Koc, DT50)	maximum daily pesticide drainage loss of a.i. in month m as a function of soil type, climate, crop, application month and compound properties [mg m^{-2}]
$relDose_c$	application rate of a.i. to crop *c*, relative to the standard rate of 1000 g ha^{-1} of the MACRO meta-model simulation [-]
MFdrain	Mitigation factor, reflecting the effects of reduction measures on pesticide drainage inputs into surface water; default = 1

Dealing with multiple applications for the input pathway drainage

Very similar methodology to FOOT-NES (cf. section 4.3.1.2)

Calculation of drainage losses and inputs

The drainage inputs calculated in section 4.3.3.1 are specific for single records in the export file delivered by the Pesticide Scenario Manager. In this file, however, it is possible that a pesticide is applied within the same polygon to the same crop more than once (either in different months or even in the same month). In contrast to drift, for the calculation of drainage (as well as runoff and erosion) inputs into surface water multiple applications to the same field cannot be treated independently of each other, since residues from one application might still be present in the field at the time of the next application. Additionally, it has to be ensured that there is no double-counting of areas in the following aggregation procedure (sections 4.3.3.3 and 4.3.3.4).

In contrast to drift, for the pathways runoff, erosion and drainage input events are triggered by rainfall events, not by pesticide application. If two applications take place in the same calendar month, it can be assumed that the pesticide runoff/erosion or drainage inputs from the two applications occur on the same day. So there is no carryover in water and sediment (because there is only one input event), but there is some carryover in the field from the first application to the second.

In FOOT-CRS, pesticide drainage inputs resulting from multiple applications (i.e. applications on the same field in different months, for instance on winter cereals in both April and November, or even in the same month) are dealt with as follows:

- If there are two or more applications in different calendar months, they are treated independently. [→ no impact on pesticide drainage loss/input calculations in the modelling module]
- If there are two or more applications in the same calendar month, we update the pesticide application rates by calculating the residues from the first application in the field and adding them to the application rate of the second application (the process is repeated for additional applications). In mathematical form:

Be there n applications, application_1 at t_1, application_2 at t_2, application_n at t_n.

For a single application, the residues from that application at time t are obtained as:

residue (t) = application_rate * exp (- ln2/DT50 * t) (eq. 4.24)

For a sequence of applications, it follows:

application_rate_2_updated = application_rate_1 * exp (- ln2/DT50 * (t_2 - t_1)) + application_rate_2 (eq. 4.25)

application_rate_3_updated = application_rate_2_updated * exp (- ln2/DT50 * (t_2 - t_1)) + application_rate_3 (eq. 4.26)

application_rate_n_updated = application_rate_n-1_updated * exp (- ln2/DT50 * (t_n – t_{n-1})) + application_rate_n. (eq. 4.27)

- Then ALL updated application rates (application rate + residues from previous applications) within each calendar month are used together with the metamodel output to calculate drainage losses and inputs (cf. section 4.3.3.1)
- For the spatial aggregation, the maximum drainage loss/input from the different applications is taken. This is appropriate because the aim of surface water exposure assessment is peak concentrations in water bodies, not average concentrations.
- However, it has additionally to be taken into account that within a polygon, the treated area fraction (Ftreated) can differ between the different applications.

Procedure to enable spatial aggregation of drainage losses and inputs

To make a correction of Ftreated for multiple applications possible at all, the following important assumption is made that application is preferential. That is, within the area of a given crop in a polygon there are areas that need treatment more regularly and more frequent than others. Examples:

- If in the first application 10 % of the area of the crop are treated, and in the second application 20 % are treated, all areas treated in the first application are treated again in the second.
- If in the first application 10 % of the area of the crop are treated, and in the second application 5 % are treated, all areas treated in the second application have also been treated in the first.

Based on this assumption, the following procedure is suggested. The procedure has to be performed for both pesticide drainage losses and inputs (the updated values from section 4.3.2.2.1).

1) All applications with the same polygon_ID/STU/cropID/year/month combination are selected. To keep the complexity of the calculations at a manageable level, the calculations are performed as if the previous applications that contributed to the updated application rates and thus to pesticide drainage losses/inputs of a particular record had the same treated area fractions as the application listed in the record (which is usually not correct, of course).

Polygon_ID	STU	cropID	Year of pest. var sw	Month of pest. var sw	appmonth	Application rate (updated)	Ftreated	Daily pesticide drainage loss/input (updated)
						g ha-1	(fraction)	mg m-2
1	1	1	95	08	4	1000	0.6	2.0
1	1	1	95	08	4	500	0.6	1.0
1	1	1	95	08	4	400	0.3	0.8
1	1	1	95	08	5	600	0.2	4.9
1	1	1	95	08	5	600	0.6	1.0
1	1	1	95	08	6	1000	0.3	6.0
1	1	1	95	08	6	1500	0.1	7.0

2) All applications with the same NUTS2/climate/SMU/CLC/STU/cropID/year/month combination are sorted in descending order of Ftreated (area fraction of crop/STU combination i that is treated with the compound of concern).

Polygon_ID	STU	cropID	Year of pest. var sw	Month of pest. var sw	appmonth	Application rate (updated)	Ftreated	Daily pesticide drainage loss/input (updated)
						g ha-1	(fraction)	mg m-2
1	1	1	95	08	4	1000	0.6	2.0
1	1	1	95	08	4	500	0.6	1.0
1	1	1	95	08	5	600	0.6	1.0
1	1	1	95	08	4	400	0.3	0.8
1	1	1	95	08	6	1000	0.3	6.0
1	1	1	95	08	5	600	0.2	4.9
1	1	1	95	08	6	1500	0.1	7.0

3) For all applications with the same polygon_ID /STU/cropID/year/month combination and the same Ftreated, the maximum drainage loss/input is taken, and the other records are deleted.

Polygon_ID	STU	cropID	Year of pest. var sw	Month of pest. var sw	appmonth	Application rate (updated)	Ftreated	Daily pesticide drainage loss/input (updated)
						g ha-1	(fraction)	mg m-2
1	1	1	95	08	4	1000	0.6	2.0
1	1	1	95	08	6	1000	0.3	6.0
1	1	1	95	08	5	600	0.2	4.9
1	1	1	95	08	6	1500	0.1	7.0

4) For all applications with the same polygon_ID/STU/cropID/percentile combination, ALL applications with smaller Ftreated AND smaller or equal drainage loss/input compared to the application with the largest Ftreated (here 0.6) are deleted. Applications with larger drainage loss/input remain unaffected.

Polygon_ID	STU	cropID	Year of pest. var sw	Month of pest. var sw	appmonth	Application rate (updated)	Ftreated	Daily pesticide drainage loss/input (updated)
						g ha-1	(fraction)	mg m-2
1	1	1	95	08	4	1000	0.6	2.0
1	1	1	95	08	6	1000	0.3	6.0
1	1	1	95	08	5	600	0.2	4.9
1	1	1	95	08	6	1500	0.1	7.0

5) Repeat procedure for the next record (i.e. the application with the 2nd largest Ftreated).

Polygon_ID	STU	cropID	Year of pest. var sw	Month of pest. var sw	appmonth	Application rate (updated)	Ftreated	Daily pesticide drainage loss/input (updated)
						g ha-1	(fraction)	mg m-2
1	1	1	95	08	4	1000	0.6	2.0
1	1	1	95	08	6	1000	0.3	6.0
1	1	1	95	08	5	600	0.2	4.9
1	1	1	95	08	6	1500	0.1	7.0

Polygon_ID	STU	cropID	Year of pest. var sw	Month of pest. var sw	appmonth	Application rate (updated)	Ftreated	Daily pesticide drainage loss/input (updated)
						g ha-1	(fraction)	mg m-2
1	1	1	95	08	4	1000	0.6	2.0
1	1	1	95	08	6	1000	0.3	6.0
1	1	1	95	08	6	1500	0.1	7.0

And so on, until there is no record left which has a smaller Ftreated AND a smaller or equal drainage loss/input than another record.

6) Finally, update each Ftreated by subtracting the next smaller Ftreated from it.

Polygon_ID	STU	cropID	Year of pest. var sw	Month of pest. var sw	appmonth	Application rate (updated)	Ftreated	Daily pesticide drainage loss/input (updated)
						g ha-1	(fraction)	mg m-2
1	1	1	95	08	4	1000	0.6 – 0.3 = 0.3	2.0
1	1	1	95	08	6	1000	0.3 – 0.1 = 0.2	6.0
1	1	1	95	08	6	1500	0.1	7.0

7) Final table

Polygon_ID	STU	cropID	Year of pest. var sw	Month of pest. var sw	appmonth	Application rate (updated)	Ftreated	Daily pesticide drainage loss/input (updated)
						g ha-1	(fraction)	mg m-2
1	1	1	95	08	4	1000	0.3	2.0
1	1	1	95	08	6	1000	0.2	6.0
1	1	1	95	08	6	1500	0.1	7.0

The sum of Ftreated in the final table (0.60) is equal to the highest Ftreated in the starting table, which is a consequence of the preferential application assumption made above. The interpretation of the final table is: 30 % of the crop area have caused a maximum daily drainage loss/input of 2.0 mg m^{-2} into surface water, 20 % have caused a maximum daily drainage loss/input of 6.0 mg m^{-2}, and 10 % a maximum daily drainage loss/input of 7.0 mg m^{-2}.

The final drainage loss/input resulting from the procedure in section 4.3.3.2 can now be used for spatial aggregation (sections 4.3.3.3 and 4.3.3.4). The drainage loss/input maps and CDF's will show maximum daily drainage losses from fields / drainage inputs into surface water from a given area for a given simulation month, NOT monthly sums of drainage losses/inputs.

The method described in 4.3.3.2 is for the option that 240 maps and 240 CDFs of drainage losses/inputs are to be created. If the user chooses a different option, the key for the query has to be adjusted.

- option “maximum losses/inputs for each of 240 simulation months” → key = Polygon_ID/STU/cropID/year/month (see above)

- option “maximum losses/inputs for each of 20 simulation years” → key = Polygon_ID /STU/cropID/year

- option “maximum losses/inputs for each of 12 calendar months” → key = Polygon_ID /STU/cropID/month

Spatial aggregation of drainage inputs to map units in FOOT-CRS (for map display)

In one FOOT-CRS run, up to 240 drainage input maps are produced (one for each month) as columns in the attribute table of a shapefile. Same methodology as in FOOT-NES (cf. section 4.3.1.2), except that FOOT-CRS uses single-part polygons and FOOT-NES multi-part polygons.

Spatial aggregation of drainage inputs to user-defined areas in FOOT-CRS (for display as CDF)

Same methodology as in FOOT-NES (cf. sections 4.3.1.4 and 4.5.5), except that the spatial aggregation is performed over the area of interest (which is equal to the catchment area in FOOT-CRS) or user-defined administrative units (NUTS2 or other).

Results from all the different relevant (i.e. with application of the pesticide of concern) polygon_ID/crop/STU combiantions represent the range of pesticide drainage inputs resulting from relevant spatial variability in the user-specified area (NUTS2, NUTS0 or NUTS2/climate/SMU/CLC polygon). However, to present these results in a valid probabilistic form we need to weight the results from each NUTS2-climate-FST-crop combination according to the area fraction covered by this combination. This will then give us the spatial probability distribution for the X^{th} (temporal) percentile PECsw. This is illustrated in the following example table (Tab. Z).
Like for the calculation of area-weighted means (cf. section 3.6.2), the following two area fractions have to be accounted for in the area-weighted averaging to obtain the area-weighted CDF:

I. area fraction of the NUTS2-climate-SMU-CLC combination (i.e. the polygon) that is covered by a particular STU/crop combination

II. area fraction of target crop in a NUTS2-climate-SMU-CLC combination that is treated with the pesticide of concern

The user will have two different options of CDF calculation

a) the statistical population of the CDF is the total area over which the aggregation is performed (AOI, NUTS2, NUTS0) [drainage: separate for the different drainage types]
b) the statistical population of the CDF is only the treated area fraction in the area over which the aggregation is performed. [drainage: separate for the different drainage types]

The two different options can lead to quite different CDF's: option a) will yield a vertically narrower CDF with an intercept. However, the curvature of the CDF's will be the same.
The relevant polygon/STU/crop combinations are determined when the user identifies an 'Area of Interest' from the GIS and enters one or more 'target crops' in the Pesticide Scenario Manager. The output from the area-of-interest selection procedure in the GIS is a shapefile, with its attribute table containing all polygons in the AOI. These polygons can then be used to select the relevant data from the FOOTPRINT agro-environmental scenario database through a query with the variables NUTS2, climate, SMU, CLC, cropID.
The area-weighted cumulative probability for each agro-environmental scenario, i.e. the "area with drainage input ≤ drainage input for the current agro-environmental scenario" is then calculated from the area represented by each agro-environmental scenario. Thus, in the example table (Tab. Z), the value for the polygon_ID/STU/crop combination that represents the 87th rank (in ascending order; 3rd in descending order) of the drainage input values of a given simulation month, the area of agro-environmental scenarios where this concentration is not exceeded is the sum of the areas of ranks 1-87. The area-weighted cumulative relative frequency of the drainage input for each unique combination is then calculated by dividing the area with drainage input ≤ drainage input of the current combination by the total area of all the combinations under the target crop(s):

cumulative rel. freq. = (area with drainage input ≤ drainage input of the current agro-env. scenario) / total area * 100 %.

*either whole area of the polygon or only treated area of the polygon

[Technical remark: If a drainage input value X occurs within the same area of aggregation more than once, the areas corresponding to this drainage input value must be added up before the ranking. Subsequently, exactly one record with the drainage input value X and the summed area is written to the ranking table.]

For each of 240 simulation months, a spatial CDF is produced.

The described methodology for calculating spatial CDF's of drainage inputs is also applicable to drainage/runoff/erosion losses from fields.

The method described in 4.3.3.4 is for the option that 240 CDFs of drainage losses/inputs are to be created. If the user chooses a different option (cf. chapter 3), the key for the query has to be adjusted.

- option "maximum losses/inputs for each of 240 simulation months" → key = Polygon_ID /STU/cropID/year/month (see Table X)

- option "maximum losses/inputs for each of 20 simulation years" → key = Polygon_ID /STU/cropID/year

- option "maximum losses/inputs for each of 12 calendar months" → key = Polygon_ID /STU/cropID/month

Polygon _ID	STU Soil Typological Unit of the SGDBE; each STU has a FST (FOOTPRINT soil type) attached to it	Crop	Polygon_ID/STU/ crop combination	Rank of drainage input value (ascending order)	Year of pest. var sw	Month of pest. var sw	Drainage input (mg/m2) [plot on x-axis of CDF]	Area represented by the NUTS/climate/ crop/STU combination [= area_polygon * I]	Treated area represented by the NUTS/climate/ crop/STU combination [= area_polygon * I * II]	Area with drainage input ≤ drainage input of the current combination (for option a, the total untreated area (difference between total area 81562800and total treated area 48937680 has to be added to the first row.	Area-weighted percentage of all unique combinations with drainage input ≤ drainage input of the current combination (area-weighted cumulative relative frequency) [plot on y-axis of CDF]
1	4410541	18	1 4410541 18	1	95	08	0.02	862210.0	517326	517326	1.06
15	4400423	18	15 4400423 18	10	95	08	0.5	2670406.0	1602243.6		33.40
14	422004	12	14 422004 12	35	95	08	6.2	4417920.8	2650752.5		98.13
16	4410546	18	16 4410546 18	87	95	08	15.1	57187.5	34312.5	48927151	99.98
16	4410596	18	16 4410596 18	88	95	08	16.8	17309.5	10385.7	48937536	99.99
16	4410549	18	16 4410549 18	89	95	08	150	239.5	143.7	48937680	100.00
							sumarea	81562800.0	48937680		

Table 5. Calculation of the Cumulative Distribution Function of drainage inputs for a user-specified area and a given percentile.
Columns highlighted in blue denote the variables used for drawing the CDF. The blue column on the right is obtained by dividing the 2nd column from the right (Area with drainage input ≤ drainage input of the current combination) by the area of aggregation (e.g. AOI; for option a, the area of aggregation is the total area (81562800 in the example); for option b, it's the total treated area (48937680 in the example)).
The resulting x,y table is exported as dbf file.

Summing up drainage inputs over the catchment area for PECsw calculation

The monthly maximum daily drainage inputs into surface water for each agro-environmental scenario $Lsw,drain\_m_{r,i}$ (calculated in section 4.3.3.1) are summed up over the catchment area:

$$Lsw,drain\_m_{catch} = \sum_r \sum_i Lsw,drain\_m_{r,i} * FcropSTU_{r,i} * Ftreated_{r,i} * A_{r,} \qquad \text{(eq. 4.28)}$$

with

$Lsw,drain\_m_{catch}$	maximum daily total drainage input of a.i. into surface water in the catchment in month m (m = 1-240) [mg]
$Lsw,drain\_m_{r,i}$	maximum daily drainage input of a.i. into surface water in month m (m = 1-240) for a given agro-env. scenario (unique combination of climate, NUTS-2 region, crop and STU) [mg m^{-2}]
STU	Soil Typological Unit of the SGDBE; each STU has a FST (FOOTPRINT soil type) attached to it
i	index of crop/STU combination (the summation is done over all crop/STU combinations in the polygon)
$FcropSTU_i$	area fraction of polygon covered by the crop/STU combination i [-]
$Ftreated_i$	area fraction of crop/STU combination i that is treated with the compound of concern [-]; this fraction only depends on the crop, not on the STU
A_r	area of the polygon [m^2]

This sum is further used for PECsw calculation. Since the $Lsw,drain\_m_{catch}$ is calculated for each month, there will be 240 PECsw,drainage values. The summation is performed analogously for pesticide inputs into surface water via interflow ($Lsw,inter\_m_{r,i}$).

A summation has also to be done for drainflow and interflow volumes, because the total drainflow and lateral subsurface flow volumes are needed later for PECsw .

$$Drainflow\_m_{catch} = \left(\sum_r \sum_i Drainflow\_m_{r,i} * FcropSTU_{r,i} * A_r\right) / 1000 \qquad \text{(eq. 4.29)}$$

[for STU's where drainflow denotes actual drainflow (drainage type DX1)]

$$\text{Interflow\_m}_{catch} = (\sum_r \sum_i \text{Interflow\_m}_{r,i} * \text{FcropSTU}_{r,i} * \text{A}_{r,}) / 1000 \qquad \text{(eq. 4.30)}$$

[for STU's where drainflow denotes lateral subsurface flow (drainage type DX2]

with

$Drainflow\_m_{catch}$	total daily drainflow volume entering the surface water network in the catchment on the day of the maximum daily pesticide drainage input in a month [m^3 d^{-1}]
$Drainflow\_m_{r,i}$	drainflow volume corresponding to $Lsw,drain\_m_{r,i}$ [mm d^{-1}]
$Interflow\_m_{catch}$	total daily interflow volume entering the surface water network in the catchment on the day of the maximum daily pesticide drainage input in a month [m^3 d^{-1}]
$Interflow\_m_{r,i}$	lateral subsurface flow volume corresponding to $Lsw,inter\_m_{r,i}$ [mm d^{-1}]
A_r	area of the polygon [m^2]
1000	unit conversion factor

4.4 Runoff and erosion inputs into surface water

4.4.1 Runoff and erosion inputs in FOOT-NES

Runoff and erosion losses and inputs for a single agro-environmental scenario and a single application

The pesticide input into surface water via runoff for a single agro-environmental scenario is calculated as follows:

Lsw,runoff_X = **{**X_runoff_loss_PRZM(FST, Climate, Crop, Appmonth, Koc, DT50) *relDose$_c$ *MFrunoff} (eq. 4.31)

where

Lsw,runoff_X	X^{th} percentile daily input of a.i. into surface waters via surface runoff for a given agro-env. scenario (unique combination of climate, NUTS-2, soil s, crop c) [mg m^{-2}]

X_runoff_loss_PRZM(FST, Climate, Crop, Appmonth, Koc, DT50)

X^{th}-percentile (of the 20-year simulation period) daily pesticide runoff loss of a.i. as a function of soil type, climate, crop, application month and compound properties [mg m^{-2}]

$relDose_{,c}$	application rate of a.i. to crop *c*, relative to the standard rate of 1000 g ha^{-1} of the PRZM meta-model simulation [-]
MFrunoff	Mitigation factor, reflecting the effects of edge-of-field reduction measures for pesticide runoff inputs into surface water [-]; default = 1

The approach for erosion is analogous to the one for surface runoff and is hence not listed here explicitly.

The pesticide runoff input calculated above feeds into the PECsw calculation routines adopted from the tool STEPS-1-2-3-4 (M. Klein, IME Schmallenberg).

Dealing with multiple applications for the input pathway runoff/erosion

Calculation of runoff and erosion losses and inputs

same methodology as for drainage (cf. section 4.3.1.2.1)

Procedure to enable spatial aggregation of runoff and erosion losses and inputs

same methodology as for drainage (cf. section 4.3.1.2.2)

Spatial aggregation of runoff and erosion inputs to map units in FOOT-NES (for map display)

In contrast to FOOT-CRS, in FOOT-NES the scenario shapefile undergoes a “dissolve” operation in the Scenario Manager (Module 2) with the variables NUTS2, climate, SMU and CLC class. As a consequence, each combination of NUTS2/climate/SMU/CLC is unique and corresponds to exactly one polygon.

For losses, inputs and PEC, the treated area fraction (iii) is accounted for during the spatial aggregation in FOOT-NES.

Results from all the different relevant (i.e. with application of the pesticide of concern) agro-environmental scenarios (NUTS2/climate/soil/crop combinations) represent the range of pesticide surface runoff inputs resulting from relevant spatial variability in the area of interest. However, for map display on polygon basis, the pesticide surface runoff inputs have to be aggregated to only one value per polygon.

Furthermore, the user has to specify in the output options of the FOOT-NES modelling module in which format he/she wants the surface runoff inputs for a polygon to be displayed:

a) area-weighted mean surface runoff inputs, referring to only the treated area

b) area-weighted mean surface runoff inputs, referring to the total polygon (unique NUTS2/climate/SMU/CLC combination) area

c) maximum surface runoff inputs occurring in the treated area (i.e. the highest PEC of all agro-environmental scenarios occurring in the NUTS/climate/SMU/CLC combination)

All three options have meaningful interpretations. However, option a) can yield much higher values than option b).

In the spatial aggregation as area-weighted mean, two area fractions have to be considered:

I) area fraction of the NUTS2-climate-SMU-CLC combination (i.e. the polygon) that is covered by a particular STU/crop combination

II) area fraction of target crop in a NUTS2-climate-SMU-CLC combination that is treated with the pesticide of concern

In reality, crops and soil types are to some degree statistically dependent (for instance, potatoes are usually not grown on heavy clays). However, given the number of FOOTPRINT crops and soil types and the fact that the dependence of the occurrence of a given crop on the soil type probably varies with climate, it is impossible to estimate crop/soil dependencies on a European level. It is therefore justifiable to assume that FOOTPRINT crops and soil types are statistically independent. Consequently, the area fraction covered by a particular STU/crop combination (i) is obtained as the product of the area fractions covered by the STU and by the crop of concern.

For the different output options, the area-specific pesticide surface runoff input for the polygon is calculated as

i) area-weighted mean surface runoff input, referring to only the treated area:

$$\mathrm{Lsw,runoff\_X_t} = \frac{\sum_i \mathrm{Lsw,runoff\_X}_i * FcropSTU_i * Ftreated_i}{\sum_i FcropSTU_i * Ftreated_i} \qquad \text{(eq. 4.32)}$$

where

STU	Soil Typological Unit of the SGDBE; each STU has a FST (FOOTPRINT soil type) attached to it
i	index of crop/STU combination (the summation is done over all crop/STU combinations in the polygon)

$FcropSTU_i$	area fraction of polygon covered by the crop/STU combination i
$Ftreated_i$	area fraction of crop/STU combination i that is treated with the compound of concern; this fraction only depends on the crop, not on the STU

ii) area-weighted mean surface runoff input, referring to the whole polygon area:

$$\text{Lsw,runoff\_X}_\text{p} = \text{Lsw,runoff\_X}_t * \frac{Atreated_{tot}}{Apolygon} \qquad \text{(eq. 4.33)}$$

where

$Atreated_{tot}$	total area in the polygon that is treated with the compound of concern
Apolygon	area of the polygon

Combining eq. 4.32 and 4.33 yields

$$\text{Lsw,runoff\_X}_\text{p} = \sum_i \text{Lsw,runoff\_X}_i * FcropSTU_i * Ftreated_i \qquad \text{(eq. 4.34)}$$

iii) maximum surface runoff input occurring in the treated area:

$$\text{Lsw,runoff\_X}_\text{m} = \max(\text{Lsw,runoff\_X}_\text{i}) \qquad \text{(eq. 4.35)}$$

The approach for erosion is analogous to the one for surface runoff and is hence not listed here explicitly.

The described aggregation methodology for pesticide runoff and erosion inputs into surface water also applies to pesticide runoff and erosion losses, of course.

Spatial aggregation of runoff and erosion inputs to user-defined areas in FOOT-NES (for display as CDF)

The methodology of CDF calculation for surface runoff or erosion inputs into surface water (or surface runoff and erosion losses) is identical to the methodology described for PECsw in section 4.5.5. The only difference is the pesticide variable to be plotted on the x-axis.

4.4.2 Runoff and erosion inputs in FOOT-FS

In FOOT-FS, runoff and erosion inputs only need to be calculated for a single agro-environmental scenario at a time. Spatial aggregation of results is therefore not necessary. Runoff and erosion inputs for a single application are calculated the same way as in FOOT-NES (cf. section 4.4.1.1).

Like in FOOT-NES, multiple applications are considered by updating the application rates with the residues present in the field from previous applications (cf. section 4.3.1.2.1). However, in contrast to FOOT-NES, where applications in different calendar months are treated as independent, in FOOT-FS residues from applications in one calendar month are carried over to applications of the same active in the next month (provided the interval between the last application in one calendar month and the first application in the following month is not longer than 28 days).

Subsequently, the highest updated application rate (application rate + residues from previous applications) within each calendar month is selected and used together with the metamodel output to calculate runoff and erosion losses and inputs (cf. section 4.4.1.1) and to run STEPS (cf. section 4.6)

4.4.3 Runoff and erosion inputs in FOOT-CRS

In FOOT-CRS, surface runoff and erosion inputs into surface water are calculated from pesticide losses using a grid-based routing procedure.

In contrast to FOOT-NES and FOOT-FS, the FOOT-CRS metamodel database does not contain 11 pesticide loss percentiles of the whole 20-year time series, but monthly maxima of pesticide loss for each month, i.e. 240 values for each simulation run (cf. chapter 2).

Runoff and erosion losses for a single agro-environmental scenario and a single application

First, pesticide surface runoff losses from fields for each agro-environmental scenario are calculated:

Loss,runoff_m = **{**m_runoff_loss_PRZM(FST, Climate, Crop, Appmonth, Koc, DT50) * $relDose_c$} (eq. 4.36)

where

Loss,runoff_m	maximum daily pesticide runoff loss of a.i. in month m for a given agro-env. scenario (unique combination of climate, NUTS-2, soil s, crop c) [mg m^{-2}]

m_runoff_loss_PRZM(FST, Climate, Crop, Appmonth, Koc, DT50)

maximum daily pesticide runoff loss of a.i. in month m as a function of soil type, climate, crop, application month and compound properties [mg m^{-2}]

$relDose_{,c}$ application rate of a.i. to crop *c*, relative to the standard rate of 1000 g ha^{-1} of the PRZM meta-model simulation [-]

The approach for erosion is analogous to the one for surface runoff and is hence not listed here explicitly.

Dealing with multiple applications for the input pathway runoff and erosion

Calculation of runoff and erosion losses

same methodology as in FOOT-NES (cf. section 4.4.1.2.1)

Procedure to enable spatial aggregation of runoff and erosion losses

same methodology as in FOOT-NES (cf. section 4.4.1.2.2)

Spatial aggregation of runoff and erosion losses to map units in FOOT-CRS (for map display)

In one FOOT-CRS run, 12, 24 or 240 drainage input maps are produced as columns in the attribute table of a shapefile. Same aggregation methodology is used as in FOOT-NES (cf. section 4.4.1.3), except that FOOT-CRS uses single-part polygons and FOOT-NES multi-part polygons. As a consequence, combinations of NUTS2/climate/SMU/CLC are not unique and one combination can correspond to several polygons.
The losses from all the different relevant (i.e. with application of the pesticide of concern) agro-environmental scenarios (NUTS2/climate/soil/crop combinations) calculated in sections 4.4.3.1 and 4.4.3.2 represent the range of pesticide surface runoff losses resulting from relevant spatial variability in the area of interest. However, for map display on polygon basis, the pesticide surface runoff inputs have to be aggregated to only one value per polygon.

Furthermore, the user has to specify in the output options of the FOOT-CRS modelling module in which format he/she wants the surface runoff inputs for a polygon to be displayed:

a) area-weighted mean surface runoff inputs, referring to only the treated area
b) area-weighted mean surface runoff inputs, referring to the total polygon area

c) maximum surface runoff inputs occurring in the treated area (i.e. the highest PEC of all agro-environmental scenarios occurring in the polygon)

All three options have meaningful interpretations. However, option a) can yield much higher values than option b).

In the spatial aggregation as area-weighted mean, two area fractions have to be considered:
I) area fraction of the NUTS2-climate-SMU-CLC combination (i.e. the polygon) that is covered by a particular STU/crop combination
II) area fraction of target crop in a NUTS2-climate-SMU-CLC combination that is treated with the pesticide of concern

In reality, crops and soil types are to some degree statistically dependent (for instance, potatoes are usually not grown on heavy clays). However, given the number of FOOTPRINT crops and soil types and the fact that the dependence of the occurrence of a given crop on the soil type probably varies with climate, it is impossible to estimate crop/soil dependencies on a European level. It is therefore justifiable to assume that FOOTPRINT crops and soil types are statistically independent. Consequently, the area fraction covered by a particular STU/crop combination (i) is obtained as the product of the area fractions covered by the STU and by the crop of concern.

For the different output options, the area-specific pesticide surface runoff input for the polygon is calculated as

i) area-weighted mean surface runoff input, referring to only the treated area:

$$\mathrm{Loss,runoff\_m_t} = \frac{\sum_i \mathrm{Loss,runoff\_m}_i * FcropSTU_i * Ftreated_i}{\sum_i FcropSTU_i * Ftreated_i} \qquad \text{(eq. 4.37)}$$

where

STU	Soil Typological Unit of the SGDBE; each STU has a FST (FOOTPRINT soil type) attached to it
i	index of crop/STU combination (the summation is done over all crop/STU combinations in the polygon)
$FcropSTU_i$	area fraction of polygon covered by the crop/STU combination i
$Ftreated_i$	area fraction of crop/STU combination i that is treated with the compound of concern; this fraction only depends on the crop, not on the STU

ii) area-weighted mean surface runoff input, referring to the whole polygon area:

$$\text{Loss,runoff\_m}_p = \text{Loss,runoff\_m}_t * \frac{Atreated_{tot}}{Apolygon} \qquad \text{(eq. 4.38)}$$

where

$Atreated_{tot}$	total area in the polygon that is treated with the compound of concern
Apolygon	area of the polygon

Combining eq. 4.37 and 4.38 yields

$$\text{Loss,runoff\_m}_p = \sum_i \text{Loss,runoff\_m}_i * FcropSTU_i * Ftreated_i \qquad \text{(eq. 4.39)}$$

iii) maximum surface runoff input occurring in the treated area:

$$\text{Loss,runoff\_m}_m = \max(\text{Loss,runoff\_m}_i) \qquad \text{(eq. 4.40)}$$

The approach for erosion is analogous to the one for surface runoff and is hence not listed here explicitly.

The described aggregation methodology for pesticide runoff and erosion losses from fields also applies to pesticide runoff and erosion inputs into surface water, of course.

Spatial aggregation of runoff and erosion losses to user-defined areas in FOOT-CRS (for display as CDF)

Same methodology as in FOOT-NES (cf. sections 4.3.1.4 and 4.6.8), except that the spatial aggregation is always performed over the area of interest (which is equal to the catchment area in FOOT-CRS).

Calculation of runoff and erosion inputs

Pesticide loss map

The polygon map of area-weighted mean losses from section 4.4.3.3. is used as the basis for the input calculatons. Although the routing is performed on a grid basis, it is not necessary to convert the pesticide losses to a grid, because it's technically only the surface runoff and eroded sediment yield that is routed (cf. following section).

Routing procedure in FOOT-CRS for surface runoff and eroded sediment

There are two different uses of the FOOT-CRS routing procedure:
a) qualitative: for updating the relative runoff and erosion classes in the map of contamination pathways → This is discussed in DL17 (François et al., 2007).
b) quantitative: for routing PRZM losses to the surface water network → This is discussed in the following in this document.

However, the routing has to be performed only 5 times (for 5 different rainfall amounts) and the resulting grids can be used for both the dominant pathways module and the modelling module.
The principle is to reduce the runoff and/or erosion value given to one cell if the contribution of this cell to the river network is limited by one or several mitigating landscape features by taking into account the infiltration or deposition processes. That is, pesticide losses from a cell are converted into pesticide inputs into surface water from this cell.
A routing approach is proposed that considers the accumulation of a theoretical initial runoff/erosion flow in the watershed, depending on the slope direction. In order to be able to take mitigating landscape features into account, the recommended analysis cell size is 10 m × 10 m.
In the routing it has to be considered that surface runoff also occurs from non-treated or even non-agricultural areas. There are three different situations:

- agricultural polygons with treated crop
- agricultural polygons without treated crop
- non-agricultural polygons (the agroenv. scenario shapefile doesn't include non-agricultural polygons; therefore, in FOOT-CRS an extra land cover map including non-agricultural parcels is needed)

It is assumed in FOOT-CRS that erosion from forest, grassland and urban areas is not significant. Erosion from non-treated areas is therefore be neglected.
For the reduction of runoff volumes, eroded sediment loads and associated pesticide losses, we use tables with reinfiltration (of surface runoff) and redeposition (of eroded particles) as function of soil, land cover, and runoff volume (Tables 6 and 7). These tables have been derived by Olivier Cerdan (BRGM) based on SCS Curve Numbers. For some land cover classes, redeposition also depends on the slope. The following rules and simplifications are used:

1. No reinfiltration takes place on arable land. This can be justified as follows: a) Infiltration will be much smaller on arable land than on forest/hedge;

b) Arable land is treated as a runoff source area (infiltration capacity is exceeded or soil is saturated) and thus cannot serve as a runoff sink at the same time. Of course, it can happen that a heavy rainstorm occurs only upslope and the soil downslope can act as a sink. But we consider that this case is less frequent than the occurrence of heavy rainfall on the entire slope.

2. We discern three types of buffers: forest, grass, shrubs
3. Deposition is treated as independent of infiltration. However, a rule is defined ensuring that deposition percentage >= infiltration percentage. This way the occurrence of sediment transport without overland flow is avoided.

Land cover	Runoff index	PRZM soil hydrologic groups				
	(mm/d)	A	B	B-C	C	D
Forest	0-3	100	99	98	97	94
	3-12	100	92	86	79	70
	12-45	100	87	78	69	58
Grass	0-3	100	99	98	96	93
	3-12	100	90	84	78	69
	12-45	100	84	76	67	56
Shrubs (macchia)	0-3	100	99	98	96	93
	3-12	100	90	84	78	69
	12-45	100	84	76	67	56
Wetlands	0-3	100	100	100	100	100
	3-12	100	100	100	100	100
	12-45	100	100	100	100	100
Other		0	0	0	0	0

Table 6 Lookup table for reinfiltration (percentage of surface flow that is intercepted)

For arable land, it is assumed that no reinfiltration takes place. For wetlands (e.g. swamps, bogs, constructed wetlands), although complete infiltration occurs, it is assumed that 40 % of dissolved pesticide entering the wetland is transported further to the surface water body in the discharge of the wetland. Since the reinfiltration values have been derived based on tabulated SCS curve numbers, the reinfiltration values are likely too high for forest (the CN implicitly include canopy interception, which does not apply in the case of surface runoff inflowing from upslope).

Land cover	Runoff index	Slope class	PRZM soil hydrologic groups				
	(mm/d)	%	A	B	B-C	C	D
Forest	0-3	n.a.	100	100	100	100	100
	3-12	n.a.	100	100	100	95	84
	12-45	n.a.	100	100	94	83	70
Grass + vineyards/orchards/hops with good grass cover between rows	0-3	n.a.	100	100	100	100	100
	3-12	n.a.	100	100	100	93	83
	12-45	n.a.	100	100	91	81	67
shrubs (macchia)	0-3	n.a.	100	99	98	96	93
	3-12	n.a.	100	90	84	78	69
	12-45	n.a.	100	84	76	67	56

Wetlands	0-3	n.a.	100	100	100	100	100
	3-12	n.a.	100	100	100	100	100
	12-45	n.a.	100	100	100	100	100
Arable land (in cropping season, with crop cover)	0-3	0-1	95	94	93	92	89
		1-2	85	84	83	82	80
		2-5	68	68	67	66	64
	3-12	0-1	95	88	82	75	67
		1-2	85	79	73	67	60
		2-5	43	39	37	34	30
	12-45	0-1	95	83	75	66	55
		1-2	85	74	67	59	49
		2-5	17	15	13	12	10
Orchards (bare soil or poor grass cover between rows	0-3	0-1	65	65	64	63	61
		1-2	55	55	54	53	52
		2-5	52	52	51	50	49
	3-12	0-1	65	60	56	51	46
		1-2	50	46	43	40	35
		2-5	32	30	28	25	22
	12-45	0-1	60	52	47	42	35
		1-2	45	39	35	31	26
		2-5	12	10	9	8	7
Vineyards and hops (bare soil or poor grass cover between rows); Arable land (outside cropping season), fallow	0-3	0-1	45	45	44	43	42
		1-2	25	25	25	24	24
		2-5	0	0	0	0	0
	3-12	0-1	35	32	30	28	25
		1-2	0	0	0	0	0
		2-5	0	0	0	0	0
	12-45	0-1	25	22	20	17	15
		1-2	0	0	0	0	0
		2-5	0	0	0	0	0
Other			0	0	0	0	0

***Table 7. Lookup table for redeposition* (percentage of sediment load that is deposited)**

For slopes > 5 % and runoff volumes > 45 mm, deposition can be assumed as zero. For wetlands (e.g. swamps, bogs, constructed wetlands), although complete deposition occurs, it is assumed that 10 % of particle-bound pesticide entering the wetland is transported further to the surface water body in the discharge of the wetland. Since the redeposition values are also dependent on the reinfiltration values (Table 6) and these have been derived based on tabulated SCS curve numbers, the redeposition values are likely too high for forest (the CN implicitly include canopy interception, which does not apply in the case of surface runoff inflowing from upslope).

The routing of surface runoff is done on a grid basis. The most convenient solution is to use a user-defined cell size for the analysis. The reinfiltration and redeposition values in Tables 6 and 7 have been derived for a grid size 10 m × 10 m. Their lower limit of applicability is a grid size of 6 m × 6 m. For grid sizes much larger than 10 m * 10 m, there are two effects:

1. the reinfiltration and redeposition values are conservative, because the same reduction applies to a larger distance
2. mitigating landscape elements like hedges, buffer strips or grassed waterways are inevitably lost.

Hence, large grid sizes will yield a worst case analysis rather than realistic inputs of surface runoff and eroded sediment into surface water. In order to be able to take into account mitigating landscape elements, the recommended analysis cell size is 10 m × 10 m. The user will get a warning that the cell size must be compatible with the size of the landscape features and that the computation time will strongly increase when the cell size is small. It is obvious that most mitigation features like edge-of-field buffers, grassed waterways or hedges can only be accounted for with a grid size of 10 m or less. Otherwise they are lost in the transformation of the landscape feature layer and the land cover map to a land cover / landscape feature grid.

To keep the calculation time at an acceptable level, the routing is not performed 240 times, but only 5 times to create the basis for interpolation. Afterwards, the 240 runoff input maps and 240 erosion input maps are obtained by interpolation. The procedure is as follows:

1. Combine landscape feature map with original Land Cover map (including non-ag. polygons) to new LC/LF layer (grid) with the rule that LF are more important than LC, discerning three types of buffers: forest, grass, shrubs
2. Use the same 5 rainfall volumes as used in the dominant pathways module to create the basis for interpolation:
   - 1st value: daily rainfall threshold for the generation of runoff for soil hydrologic group D, fallow condition, antecedent moisture condition II (CN = 94)
   - 2nd value: 90th percentile daily rainfall volume of the 20-year time series of the respective FOOTPRINT climate zone (FCZ). The percentile only refers to the days where rainfalls occurs, not to the whole 20 years.
   - 3rd value: 95th percentile daily rainfall volume of the 20-year time series of the FCZ
   - 4th value: 99th percentile daily rainfall volume he 20-year time series of the FCZ
   - 5th value: max. daily rainfall of the 20-year time series of the FCZ.
3. calculate (area-weighted) initial runoff volume using Curve Numbers specific for soil hydrologic group and CLC class.
   - CN are also needed for non-agricultural CLC classes (forest, urban, etc.).
   - Possibly also consider dry and moist antecedent soil moisture conditions or crop vs. no crop.
   - need to distinguish in CN for the relevant CLC classes between vines with grass and vines without or with only poor grass cover (same for orchards, olives, hops)

4. The routing is then performed in FOOT-CRS according to Fig. 2 (runoff) and Fig. 3 (erosion), using the reinfiltration and deposition values of Tables 6 and 7. The results are
   - 5 grids with "fraction of runoff volume reaching surface water" → average over polygon using zonal statistics → 5 values for each polygon
   - 5 grids with "fraction of eroded sediment reaching surface water" → average over polygon using zonal statistics → 5 values for each polygon
5. Query the rainfall volume corresponding to the max. daily pesticide runoff loss for a given month in the metamodel database, calculate area-weighted average over polygon (area-weighted average rainfall is to be used because different rainfall amounts for different STUs in the same polygon would be illogical)
6. From rainfall, compute area-weighted initial runoff volume using Curve Numbers specific for soil hydrologic group and CLC class for each scenario polygon (weighting based on the area fractions covered by the different STU's in the SMU).
7. Calculate area-weighted average pesticide runoff and erosion loss for the polygon; the area-weighting is based on area fraction covered by an STU in the SMU
8. Interpolate linearly for each polygon, using 240 rainfall volumes
   - initial runoff volume (240 values)
   - fraction of runoff and pesticide runoff loss reaching sw (240 values)
   - fraction of eroded sediment and pesticide erosion loss reaching sw (240 values)
9. Multiply the pesticide runoff and erosion losses (shapefile) with the fractions of pesticide runoff loss and erosion loss, resp., reaching surface water → pesticide runoff and erosion input maps (shapefiles)
10. Multiply the initial runoff volumes (shapefile) with the fractions of surface runoff volume reaching surface water → surface runoff flow input map (shapefile)

The resulting pesticide input maps are further aggregated to spatial CDF's and to total inputs into surface water in the catchment (which are used for PECsw calculation). Also the surface runoff flow input map is summed up to total surface runoff volume reaching the river ($Runoff\_m_{catch}$).

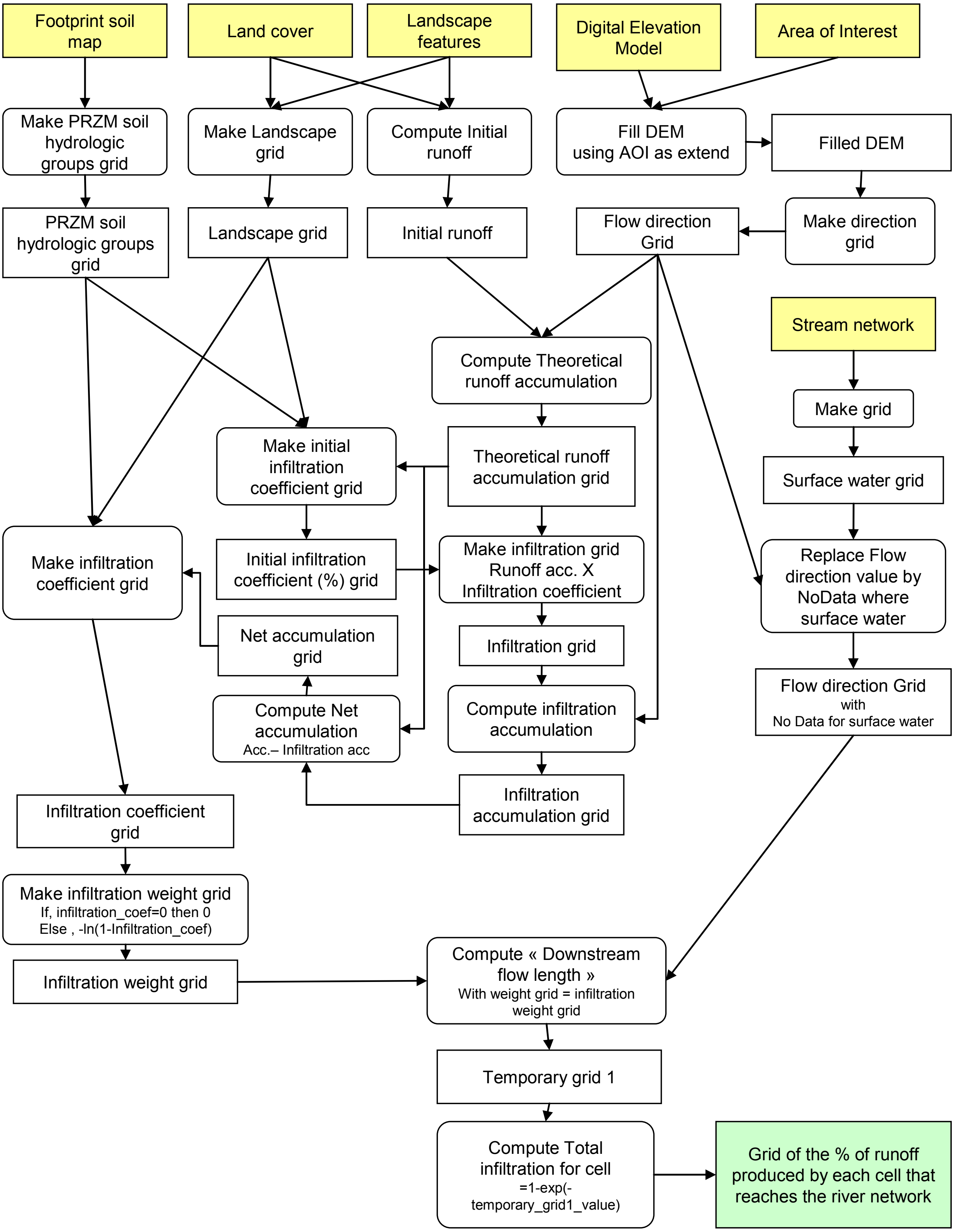

Fig. 2. Flow chart to be used in FOOT-CRS for mapping the percentage of runoff that reaches the surface water

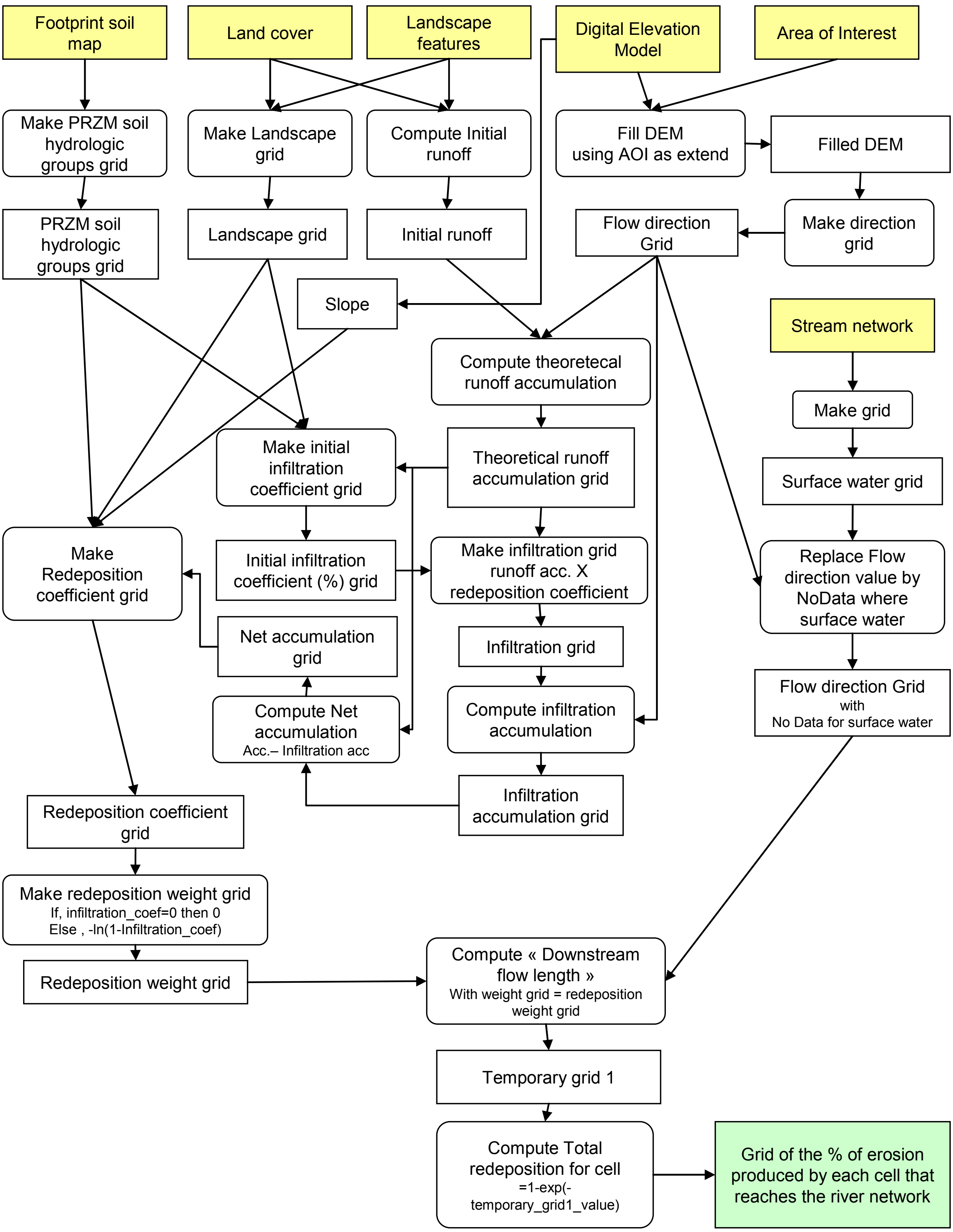

Fig. 3 Flow chart to be used in FOOT-CRS for mapping the percentage of eroded sediment that reaches the surface water

Discussion: Choice of PRZM losses to be stored in the MM database

(The discussion equally applies to MACRO drainage losses, although there is no routing needed there)

There has been and much discussion about which events / percentiles to extract and distribute from PRZM 20 year time series.

1. The problem

The basic problem in FOOT-CRS is that we are aggregating pesticide inputs into surface water over space. That means, we must avoid that the input grid for the routing contains losses that do not coincide in time, i.e. that occur on different days or even in different months.

There are several source of spatial variability of the occurrence date of an X^{th} percentile loss event (as used in FOOT-NES and FOOT-FS) in the catchment:

i) **spatial variable weather:** In reality, rainstorms may occur only in parts of the catchment. In FOOTPRINT, most catchment will only have one climate zone (and thus have the same weather time series over the whole catchment), but there will obviously be some catchments with 2 or 3 climate zones (and thus different weather time series).

ii) **spatial variability of application dates:** In reality, on two adjacent fields with the same crop/pesticide/application month combination, in the same year one field may be sprayed, for instance, on the 10^{th} of April and the other on the 15^{th}, i.e. 5 days later. In FOOTPRINT, the application date is connected to the weather file. If the catchment has only one climate zone, application on the same crop will occur on the same day in the whole catchment (clearly unrealistic, of course)

iii) **different soils:** even for the same crop, application date and pesticide, the X^{th} percentile loss event might not coincide on different soils.

iv) **different crops:** different crops often have different application dates and different timing of crop growth stages. So the X^{th} percentile losses between different crops, even for the same soil, will probably not coincide.

To overcome at least problems iii) and iv), we do not store X^{th} percentile losses of the whole time series in the FOOT-CRS metamodel database, but we store maximum daily losses for each month and use them for calculation of pesticide inputs and PECsw. The 240 different PECsw are then ranked and a temporal CDF and return periods of given events are calculated.

Advantages:

- It can be assumed as a first approximation that the maximum daily loss in a given month occurs on the same day in a catchment (at least this is much more probable than the coincidence of an X^{th} percentile loss of the whole time series in the catchment)
- The PECsw cumulative probabilities already account for runoff volumes and month-specific discharges.
- The method also works for more than one crop at the same time!

Disadvantages:

- Information on all events in a month smaller than the highest is lost
  → seasonality problem: the 2^{nd} or 3^{rd} highest loss in month X may be higher than the highest loss in month Y
  → no statements for return periods less than 1 month possible

In our opinion, the advantages of the proposed approach clearly outweigh the disadvantages.

4.5 PEC calculation for edge-of-field water bodies (FOOT-NES)

4.5.1 PECsw and PECsed for single agro-environmental scenarios

Compared to FOOT-CRS, calculation of Predicted Environmental Concentrations in surface water (PECsw) and risk assessment are relatively straightforward in FOOT-NES and FOOT-FS, since only „edge-of-field" water bodies are considered. However, FOOT-NES must also be able to provide time-weighted average concentrations (TWAC) in surface water to enable comparison with certain ecotoxicological thresholds.

In the FOOT tools, loads and PECsw/PECsed are estimated separately for drift, runoff + erosion, and drainage. For instance, surface runoff might lead to higher peak concentrations, but to less frequent exceedances of a given ecotoxicological threshold concentration than drift inputs. Having the PEC separately for each pathway will also make it easier to recommend mitigation measures and evaluate their effect at the national and EU scale. This approach is justified because a coincidence of peak concentrations from the different input pathways on the same day is not realistic.

In FOOT-NES, we focus on edge-of-field water bodies and follow an approach similar to FOCUSsw (step 3), including the conceptual (but clearly not real) upstream catchment inputs to the FOCUS water bodies. The purpose of these in FOCUSsw was simply to provide what was estimated to be a realistic time series of water and pesticide fluxes from the upstream catchment into the surface water body.

We need the FOOT-NES model output to be driven by actual field level application rates and meta-model calculations for each relevant agro-environmental scenario (NUTS2-climate-FST-crop combination) in the area of interest. This will give the (temporal) X^{th} percentile edge-of-field losses for each relevant agro-environmental scenarios in the area of interest. Meta-modelling results are then fed into PECsw calculation equations adopted from the STEPS-1-2-3-4 model (Klein, 2007). The advantage of calculating PECsw/PECsed separately for each agro-environmental scenario is that, because we are dealing with only one climate, soil type and crop, the water fluxes are consistent over the entire catchment of the edge-of-field water body. This makes it possible to upscale water and (for the stream scenario) pesticide fluxes from the field adjacent to the water body to the upstream catchment), like it is done in FOCUSsw.

In the following, the choice of MACRO and PRZM loss percentiles to be stored in the meta-model database for input into PEC calculation with the STEPS-1-2-3-4 equations is explained. In contrast to PEC calculation in FOOT-CRS, there is no problem with seasonality or non-coincidence of X^{th} percentile events here, because we first calculate PEC for each agro-environmental scenario and then do spatial aggregation.

Since we go for percentiles of the whole time series, it has to be higher percentiles, because the lower 80 or 90 percent may all be zero loss (no drainage or runoff inputs at all). The percentiles to be stored in the Metamodel Database are:

(percentiles of the whole time series, with return period in parentheses)
90^{th} (10 days)
95^{th} (20 days)
96.7^{th} (30 days)
98.0^{th} (50 days),
98.7^{th} (75 days)
99.0^{th} (100 days)
99.33^{th} (150 days)
99.50^{th} (200 days)
99.73^{th} (1 year)
99.90^{th} (3 years; though already very uncertain)
99.97^{th} (10 years; very uncertain)
→ 11 figures

We store selected percentiles of the whole 20 year time series rather than percentiles of annual maxima here, because from an ecological point of view, it is important to have information on concentrations in surface water not only for longer return periods (which are relevant for acute toxicity), but also for shorter return periods (which are relevant for recovery and chronic toxicity).
Of course, an X^{th} percentile runoff or drainage loss does not correspond exactly to an X^{th} percentile PECsw, because associated water volumes vary from event to event, and the base flow varies on a monthly basis. However, since it is not possible to store the entire 20 year MACRO and PRZM output time series on the FOOTPRINT distribution DVD due to storage space limitations, it can be considered an acceptable first approximation to assume that an X^{th} percentile loss event translates to an X^{th} percentile PECsw (if there are no mitigation measures implemented with seasonally variable efficiency).

STEPS-1-2-3-4 (Klein, 2007a) is an upgrade of the STEPS-1-2-calculator used in the lower tier calculations of the FOCUSsw scenarios (FOCUS, 2001). STEP-3, whose equations are used in FOOT-FS and FOOT-NES, was created as a quick replacement of the very complex and computation-intensive TOXSWA model (FOCUS, 2001). While being much faster, STEP-3 yields almost the same results as TOXSWA (Klein, 2007b). STEP-3 simulates a water-sediment system, with the sediment being split into an upper and a lower layer. It works on an hourly basis and goes through a loop in each simulation hour. Within a loop, STEP-3 sequentially simulates all transport and transformation processes (water inflow, complete mixing of the water column, diffusive exchange between water column and sediment and between the two sediment layers, pesticide sorption and degradation, water outflow).
Within FOOTPRINT, the STEPS-1-2-3-4 calculation is run for 28 consecutive days. On the first day, the pesticide inputs from the MACRO or PRZM metamodel or from the drift calculations are added. The following days are run with zero inputs of pesticide and runoff/drainflow.The STEPS-1-2-3-4 algorithms produce both
a) initial PECsw and PECsed and
b) time weighted average concentrations (TWAC) over user-specified periods from 1 to 28 days.

As explained above, PECsw/PECsed are assessed separately for each pathway (drift, drainage, runoff/erosion). For scenarios where subsurface lateral flow occurs, the X^{th} percentile pesticide loss via subsurface flow calculated with MACRO (i.e. emulated with primary drains) and corresponding flow volume is added to the PECsw calculations for the pathway runoff and erosion.

In FOOT-NES the PEC have to be spatially aggregated for display as map and as CDF.

In the Pesticide Scenario Manager, the FOOT-NES user has the opportunity to select more than one percentile (or even all 11 percentiles available in the metamodel database) of the 20-year PRZM/MACRO loss time series. The different selected percentiles will then be displayed as separate maps or as separate spatial cumulative distribution functions (CDF).

4.5.2 FOOT-NES: Dealing with multiple applications for PECsw/sed due to spray drift inputs

Calculation of PECsw/sed due to spray drift inputs

The PECsw/sed,drift calculated in section 4.5.1 are specific for single records in the export file delivered by the Pesticide Scenario Manager. In this file, however, it is possible that a pesticide is applied within the same polygon to the same crop more than once (either in different months or even in the same month). When calculating PECsw/sed due to drift, multiple applications cannot be treated independently any more, because concentrations will be underestimated if at the time of application there are residues from previous application.left in the water/sediment system.

In FOOT-NES, PECsw/sed,drift resulting from multiple applications (i.e. applications on the same field in different months, for instance on winter cereals in both April and November, or even in the same month) are dealt with as follows:

- Each application (active substance) is assessed individually in STEPS. The residues in the water/sediment system from the n^{th} application at the time of the $n+1^{th}$ application following application feed into the STEPS run for the $n+1^{th}$ application. The interval between applications is known because the user also enters the application day in the Pesticide Scenario Manager.
- For the spatial aggregation, the highest PECsw (analogously: PECsed, TWACsw, TWACsed) of the PECsw calculated in the different simulation runs for a particular application month is taken as the final PECsw for this application month ("PECsw,drift,final" in the following). This is appropriate because the aim of surface water exposure assessment is peak concentrations in water bodies, not average concentrations.
- However, it has additionally to be taken into account that within a polygon, the treated area fraction (Ftreated) can differ between the different applications.

Procedure to enable spatial aggregation of PECsw/sed due to spray drift inputs

To make a correction of Ftreated for multiple applications possible at all, the following important assumption is made that application is preferential. That is, within the area of a given crop in a polygon there are areas that need treatment more regularly and more frequent than others. Examples:

- If in the first application 10 % of the area of the crop are treated, and in the second application 20 % are treated, all areas treated in the first application are treated again in the second.
- If in the first application 10 % of the area of the crop are treated, and in the second application 5 % are treated, all areas treated in the second application have also been treated in the first.

Based on this assumption, the following procedure is suggested (example for PECsw, but same methodology applies to PECsed, TWACsw, TWACsed):

1) All applications with the same NUTS2/climate/SMU/CLC/STU/cropID/percentile combination are selected. (Drift is independent of soil and thus STU, but the STU is part of the key identifying a record in the result table. The drift percentile is a constant within a FOOT-NES run, but to maintain consistency with the calculations for drainage/runoff/erosion, the drift percentile is used here in the key.)

NUTS2	climate	SMU	CLC	STU	cropID	per-centile	appmonth	Appli-cation rate g ha-1	Ftreated (fraction)	PECsw, drift,final µg L-1
1	1	1	1	1	1	90	3	1000	0.6	2.0
1	1	1	1	1	1	90	4	500	0.5	1.0
1	1	1	1	1	1	90	4	400	0.3	0.8
1	1	1	1	1	1	90	5	600	0.2	4.9
1	1	1	1	1	1	90	5	600	0.6	1.0
1	1	1	1	1	1	90	6	1000	0.3	6.0
1	1	1	1	1	1	90	6	1500	0.1	7.0

2) All applications with the same NUTS2/climate/SMU/CLC/STU/cropID/percentile combination are sorted in descending order of Ftreated (area fraction of crop/STU combination i that is treated with the compound of concern).

NUTS2	climate	SMU	CLC	STU	cropID	per-centile	appmonth	Appli-cation rate	Ftreated	PECsw, drift,final
								g ha-1	(fraction)	µg L-1
1	1	1	1	1	1	90	3	1000	0.6	2.0
1	1	1	1	1	1	90	5	600	0.6	1.0
1	1	1	1	1	1	90	4	500	0.5	1.0
1	1	1	1	1	1	90	4	400	0.3	0.8
1	1	1	1	1	1	90	6	1000	0.3	6.0
1	1	1	1	1	1	90	5	600	0.2	4.9
1	1	1	1	1	1	90	6	1500	0.1	7.0

3) For all applications with the same NUTS2/climate/SMU/CLC/STU/cropID/percentile combination and the same Ftreated, the maximum PECsw is taken, and the other records are deleted.

NUTS2	climate	SMU	CLC	STU	cropID	per-centile	appmonth	Appli-cation rate	Ftreated	PECsw, drift,final
								g ha-1	(fraction)	µg L-1
1	1	1	1	1	1	90	3	1000	0.6	2.0
1	1	1	1	1	1	90	4	500	0.5	1.0
1	1	1	1	1	1	90	6	1000	0.3	6.0
1	1	1	1	1	1	90	5	600	0.2	4.9
1	1	1	1	1	1	90	6	1500	0.1	7.0

4) For all applications with the same NUTS2/climate/SMU/CLC/STU/cropID/percentile combination, ALL applications with smaller Ftreated AND smaller or equal PECsw,drift,final compared to the application with the largest Ftreated (here 0.6) are deleted. Applications with larger PECsw,drift,final remain unaffected.

NUTS2	climate	SMU	CLC	STU	cropID	per-centile	appmonth	Appli-cation rate	Ftreated	PECsw, drift,final
								g ha-1	(fraction)	µg L-1
1	1	1	1	1	1	90	3	1000	0.6	2.0
1	1	1	1	1	1	90	4	500	0.5	1.0
1	1	1	1	1	1	90	6	1000	0.3	6.0
1	1	1	1	1	1	90	5	600	0.2	4.9
1	1	1	1	1	1	90	6	1500	0.1	7.0

NUTS2	Climate	SMU	CLC	STU	cropID	per-centile	appmonth	Appli-cation rate	Ftreated	PECsw, drift,final
								g ha-1	(fraction)	µg L-1
1	1	1	1	1	1	90	3	1000	0.6	2.0
1	1	1	1	1	1	90	6	1000	0.3	6.0
1	1	1	1	1	1	90	5	600	0.2	4.9
1	1	1	1	1	1	90	6	1500	0.1	7.0

5) Repeat procedure for the next record (i.e. the application with the 2nd largest Ftreated).

NUTS2	Climate	SMU	CLC	STU	cropID	per-centile	appmonth	Application rate g ha-1	Ftreated (fraction)	PECsw, drift,final µg L-1
1	1	1	1	1	1	90	3	1000	0.6	2.0
1	1	1	1	1	1	90	6	1000	0.3	6.0
1	1	1	1	1	1	90	5	600	0.2	4.9
1	1	1	1	1	1	90	6	1500	0.1	7.0

NUTS2	Climate	SMU	CLC	STU	cropID	per-centile	appmonth	Application rate g ha-1	Ftreated (fraction)	PECsw, drift,final µg L-1
1	1	1	1	1	1	90	3	1000	0.6	2.0
1	1	1	1	1	1	90	6	1000	0.3	6.0
1	1	1	1	1	1	90	6	1500	0.1	7.0

And so on, until there is no record left which has a smaller Ftreated AND a smaller or equal PECsw,drift,final than another record.

6) Finally, update each Ftreated by subtracting the next smaller Ftreated from it.

NUTS2	Climate	SMU	CLC	STU	cropID	per-centile	appmonth	Application rate g ha-1	Ftreated (fraction)	PECsw, drift,final µg L-1
1	1	1	1	1	1	90	3	1000	0.6 – 0.3 = 0.3	2.0
1	1	1	1	1	1	90	6	1000	0.3 – 0.1 = 0.2	6.0
1	1	1	1	1	1	90	6	1500	0.1	7.0

7) Final table

NUTS2	Climate	SMU	CLC	STU	cropID	per-centile	appmonth	Application rate g ha-1	Ftreated (fraction)	PECsw, drift,final µg L-1
1	1	1	1	1	1	90	3	1000	0.3	2.0
1	1	1	1	1	1	90	6	1000	0.2	6.0
1	1	1	1	1	1	90	6	1500	0.1	7.0

The sum of Ftreated in the final table (0.60) is equal to the highest Ftreated in the starting table, which is a consequence of the preferential application assumption made above. The interpretation of the final table is: 30 % of the crop area have caused a maximum PECsw,drift, final of 2.0 µg L-1 into surface water, 20 % have caused a maximum PECsw,drift,final of 6.0 µg L-1, and 10 % a max. PECsw,drift,final of 7.0 µg L-1.

The final PECsw,drift table resulting from the procedure in section 4.5.2 can now be used for spatial aggregation (sections 4.5.4 and 4.5.5).

The methodology described in this section (4.5.2.2) is identical to the one described for drift inputs (section 4.2.1.2.2). The algorithms from 4.2.1.2.2 can therefore be adopted without modification.

4.5.3 FOOT-NES: Dealing with multiple applications for PECsw/sed due to drainage or runoff/erosion inputs

Calculation of PECsw/sed due to drainage or runoff/erosion inputs

For the input pathways drainage and runoff/erosion, multiple applications in the same calendar month are already dealt with before running STEPS by adjusting the pesticide application rates (cf. section 4.3.1.2.1). Therefore, the PECsw (analogously: PECsed, TWACsw, TWACsed) due to drainage or runoff/erosion inputs calculated with STEPS (cf. section 4.5.1) do not need further adjustments.

- For the spatial aggregation, the highest PECsw (analogously: PECsed, TWACsw, TWACsed) of the PECsw calculated in the different simulation runs for a particular application month is taken as the final PECsw for this application month ("PECsw,final" in the following). This is appropriate because the aim of surface water exposure assessment is peak concentrations in water bodies, not average concentrations.
- However, it has additionally to be taken into account that within a polygon, the treated area fraction (Ftreated) can differ between the different applications.

Procedure to enable spatial aggregation of PECsw/sed due to drainage or runoff/erosion

Same methodology as in 4.5.2.2 (PECsw/sed,drift) and 4.2.1.2.2 (drift inputs)

4.5.4 Spatial aggregation of PECsw and PECsed to map units in FOOT-NES (for map display)

Results from all the different relevant (i.e. with application of the pesticide of concern) agro-environmental scenarios (NUTS2/climate/soil/crop combinations) represent the range of

PECsw/PECsed resulting from relevant spatial variability in the area of interest. However, for map display on polygon basis, the PEC have to be aggregated to only one value per polygon.

Furthermore, the user has to specify in the output options of the FOOT-NES modelling module in which format he/she wants the PEC for a polygon to be displayed:

a) area-weighted mean PEC, referring to only the treated area
b) area-weighted mean PEC, referring to the total polygon (unique NUTS2/climate/SMU/CLC combination) area
c) maximum PEC occurring in the treated area (i.e. the highest PEC of all agro-environmental scenarios occurring in the NUTS/climate/SMU/CLC combination)

All three options have meaningful interpretations. However, option a) can yield much higher values than option b).

In the spatial aggregation as area-weighted mean, two area fractions have to be considered:

I. area fraction of the NUTS2-climate-SMU-CLC combination (i.e. the polygon) that is covered by a particular STU/crop combination

II. area fraction of target crop in a NUTS2-climate-SMU-CLC combination that is treated with the pesticide of concern

In reality, crops and soil types are to some degree statistically dependent (for instance, potatoes are usually not grown on heavy clays). However, given the number of FOOTPRINT crops and soil types and the fact that the dependence of the occurrence of a given crop on the soil type probably varies with climate, it is impossible to estimate crop/soil dependencies on a European level. It is therefore justifiable to assume that FOOTPRINT crops and soil types are statistically independent. Consequently, the area fraction covered by a particular STU/crop combination (i) is obtained as the product of the area fractions covered by the STU and by the crop of concern.

For the different output options, the PECsw (or PECsed, TWACsw, TWACsed) for the polygon is calculated as

i) area-weighted mean PEC, referring to only the treated area:

$$\mathrm{PECsw}_t = \frac{\sum_i PEC_i * FcropSTU_i * Ftreated_i}{\sum_i FcropSTU_i * Ftreated_i} \qquad \text{(eq. 4.41)}$$

where

STU	Soil Typological Unit of the SGDBE; each STU has a FST (FOOTPRINT soil type) attached to it
i	index of crop/STU combination (the summation is done over all crop/STU combinations in the polygon)
$FcropSTU_i$	area fraction of polygon covered by the crop/STU combination i
$Ftreated_i$	area fraction of crop/STU combination i that is treated with the compound of concern; this fraction only depends on the crop, not on the STU

ii) area-weighted mean PEC, referring to the whole polygon area:

$$\mathrm{PECsw}_{\mathrm{p}} = PECsw_t * \frac{Atreated_{tot}}{Apolygon} \qquad \text{(eq. 4.42)}$$

where

$Atreated_{tot}$	total area in the polygon that is treated with the compound of concern
Apolygon	area of the polygon

Combining eq. 4.41 and 4.42 yields

$$\mathrm{PECsw}_{\mathrm{p}} = \sum_i PEC_i * FcropSTU_i * Ftreated_i \qquad \text{(eq. 4.43)}$$

iii) maximum PEC occurring in the treated area:

$$PECsw_m = \max (PECsw_i) \qquad \text{(eq. 4.44)}$$

4.5.5 Spatial aggregation of PECsw and PECsed to user-defined areas in FOOT-NES (for display as CDF)

Results from all the different relevant (i.e. with application of the pesticide of concern) agro-environmental scenarios (NUTS2-climate-soil-crop combinations) represent the range of PEC resulting from relevant spatial variability in the user-specified area (NUTS2, NUTS0 or NUTS2/climate/SMU/CLC polygon). However, to present these results in a valid probabilistic form we need to weight the results from each NUTS2/climate/soil/crop combination according to the area fraction covered by this combination. This will then give us the spatial probability distribution for the X^{th} (temporal) percentile PECsw. This is illustrated in the following example table (Tab. Z).

Like for the calculation of area-weighted means (cf. section 3.6.2), the following two area fractions have to be accounted for in the area-weighted averaging to obtain the area-weighted CDF:

I. area fraction of the NUTS2/climate/SMU/CLC combination (i.e. the polygon) that is covered by a particular STU/crop combination

II. area fraction of target crop in a NUTS2/climate/SMU/CLC combination that is treated with the pesticide of concern

The user will have two different options of CDF calculation

a) the statistical population of the CDF is the total area over which the aggregation is performed (AOI, NUTS2, NUTS0) [in case of PECdrainage: only the area is included where actual drainflow is modelled]

b) the statistical population of the CDF is only the treated area fraction in the area over which the aggregation is performed. [in case of PECdrainage: only the area is included where actual drainflow is modelled]

The two different options can lead to quite different CDF's: option a) will yield a vertically narrower CDF with an intercept. However, the curvature of the CDF's will be the same.

The relevant agro-environmental scenarios (NUTS2-climate-STU-crop combinations) are determined when the user identifies an 'Area of Interest' from the GIS and enters one or more 'target crops' in the Pesticide Scenario Manager. The output from the area-of-interest selection procedure in the GIS is a shapefile, with its attribute table containing all NUTS, climate, SMU and CLC code combinations in the AOI. These combinations can then be used to select the relevant data from the FOOTPRINT agro-environmental scenario database through a query with the variables NUTS2, climate, SMU, CLC, cropID.

The area-weighted cumulative probability for each agro-environmental scenario, i.e. the "area with PEC ≤ PEC for the current agro-environmental scenario" is then calculated from the area represented by each agro-environmental scenario. Thus, in the example table (Tab. 8), the value for the NUTS2-climate-STU-crop combination that represents the 87^{th} rank (in ascending order; 3^{rd} in descending order) of the (temporal) 95^{th} percentile PEC values, the area of agro-environmental scenarios where this concentration is not exceeded is the sum of the areas of ranks 1-87. The area-weighted cumulative relative frequency of the PEC for each unique combination is then calculated by dividing the area with PEC ≤ PEC of the current combination by the total area of all the combinations under the target crop(s):

cumulative rel. freq. = (area with PEC ≤ PEC of the current agro-env. scenario) / total area * 100 %.

*either whole area of the polygon or only treated area of the polygon

[Technical remark: If a PEC value X occurs within the same area of aggregation more than once, the areas corresponding to this PEC value must be added up before the ranking. Subsequently, exactly one record with the PEC value X and the summed area is written to the ranking table.]

For each temporal percentile selected in the pesticide scenario manager, a spatial CDF is produced. Spatial and temporal variability are kept strictly separate. The main reason why one should keep temporal and spatial variability separate is: Upon merging spatial and temporal variability, valuable information is lost. The ecological interpretation for the case “threshold is exceeded 100 % of the time in 50 % of the area” would be very different from “threshold is exceeded 50 % of the time in 100 % of the area”. (cf. Verdonck, 2003). After merging spatial and temporal variability, one could not distinguish these two extreme cases any more.

The described methodology for calculating spatial CDF’s of PECsw is also applicable to PECsed, TWACsw, TWACsed, PECgw, pesticide runoff/erosion/drainage inputs into surface water as well as pesticide runoff/erosion/drainage losses from fields.

NUTS 2	climate	STU Soil Typological Unit of the SGDBE; each STU has a FST (FOOTPRINT soil type) attached to it	Crop	NUTS2-climate-STU-crop combination	PEC rank (ascending order)	(temporal) percentile	PEC (µg/L) [plot on x-axis of CDF]	area represented by the NUTS/climate/ crop/STU combination [= area_polygon * I]	Treated area represented by the NUTS/climate/ crop/STU combination [= area_polygon * I * II]	Area with PEC ≤ PEC of the current combination (for option a, the total untreated area (difference between total area 81562800and total treated area 48937680 has to be added to the first row.	Area-weighted percentage of all unique combinations with PEC ≤ PEC of the current combination (area-weighted cumulative relative frequency) [plot on y-axis of CDF]
342	16	4410541	18	342 16 4410541 18	1	95	0.02	862210.0	517326	517326	1.06
326	15	4400423	18	326 15 4400423 18	10	95	0.5	2670406.0	1602243.6		33.40
306	14	422004	12	306 14 422004 12	35	95	6.2	4417920.8	2650752.5		98.13
342	16	4410546	18	342 16 4410546 18	87	95	15.1	57187.5	34312.5	48927151	99.98
342	16	4410596	18	342 16 4410596 18	88	95	16.8	17309.5	10385.7	48937536	99.99
342	16	4410549	18	342 16 4410549 18	89	95	150	239.5	143.7	48937680	100.00
							sumarea	81562800.0	48937680		

Table 8. Calculation of the Cumulative Distribution Function of PECsw/PECsed for a user-specified area and a given percentile. Columns highlighted in blue denote the variables used for drawing the CDF. The blue column on the right is obtained by dividing the 2nd column from the right (Area with PEC ≤ PEC of the current combination) by the area of aggregation (e.g. NUTS2 unit; for option a, the area of aggregation is the total area (81562800 in the example); for option b, it's the total treated area (48937680 in the example)). The resulting x,y table is exported as dbf file.

4.6 PEC calculation for edge-of field water bodies (FOOT-FS)

In FOOT-FS, PECsw/sed only need to be calculated for a single agro-environmental scenario at a time. Spatial aggregation of results is therefore not necessary. PECsw/sed for a single agro-environmental scenario are calculated the same way as in FOOT-NES. However, it has to be kept in mind that for the pathways runoff/erosion and drainage there are differences between FOOT-FS and FOOT-NES in the updating of pesticide application rates in case of multiple applications (cf. sections 4.3.2 and 4.4.2).

4.7 PEC calculation for the catchment outlet (FOOT-CRS)

Calculation of Predicted Environmental Concentrations in surface water (PECsw) and risk assessment are relatively straightforward in FOOT-FS und FOOT-NES, since only „edge-of-field“ water bodies are considered. In FOOT-CRS however, which operates at the catchment scale, the aim is concentrations at the outlet, or even exceedance frequencies of x µg L^{-1} (usually 0.1 µg L^{-1}) in a given period. This implies that results must be aggregated meaningfully. The following phenomena must be considered at the catchment scale:

- different flow lengths and travel times from each field to the catchment outlet („geomorphological dispersion“)
- transport and dispersion in the water course
- sorption and degradation during transport in the water course
- spatial and temporal variability of weather and application dates

The standard version of the Gustafson equation (which is used to account for geomorphological dispersion; cf. Gustafson et al., 2004) does not account for sorption and degradation yet. Therefore, pesticide sorption and degradation during transport in the water course are (conservatively) neglected at least in the first version of FOOT-CRS. Interaction between water column and sediment is handled in a strongly simplifying, but conservative way with respect to PECsw:

- The fraction of particle-bound pesticide inputs that is transported downstream from its point of entry is estimated with a simple approach assuming instantaneous sorption equilibrium at the point of entry between the flowing water body and the bed sediment and neglecting sediment pore water. During the downstream transport of this fraction, no more interaction with the bed sediment is considered.

- For pesticide inputs into the water column (drift, drainage, surface runoff, lateral subsurface flow), no interaction with the bed sediment is considered.

It is proposed to estimate loads and PECsw at the catchment outlet separately for the input pathway drift and offer different options for combination of PEC for drainage, lateral subsurface flow and runoff/erosion (as opposed to add up drift and drainage or drift and runoff/erosion like in FOCUS (2001)). For instance, surface runoff might lead to higher peak concentrations at the outlet, but to less frequent exceedances of 0.1 µg L^{-1} than drift inputs. Having separate PEC will also make it easier to recommend mitigation measures and evaluate their effect at the catchment scale. This approach is justified because a coincidence of peak concentrations from drift and the other input pathways on the same day is not realistic. The different PECsw equations are described in the following.

4.7.1 PECsw equations

PECsw due to spray drift inputs

$$PECsw,drift\_X = Lsw,drift\_X_{catch} / Q_{mean} * GF \quad \text{(eq. 4.45)}$$

where

PECsw,drift_X	X^{th} percentile daily PECsw at the catchment outlet resulting from spray drift inputs [mg m^{-3}], for a given application date
$Lsw,drift\_X_{catch}$	daily total drift input into surface water in the catchment at a given application date [mg d^{-1}].
Q_{mean}	month-specific mean daily river discharge at the catchment outlet [m^3 d^{-1}]
GF	Peak Concentration Reduction Factor from Gustafson equation [-]. The Gustafson equation (cf. section 4.7.3) converts a pulse input into a breakthrough curve at the catchment outlet, using the mean river length in the catchment (computed from surface water network) and a generic mean streamflow velocity → The peak concentration at the outlet will be lower than “total input / discharge”.

Note that PECsw,drift are calculated for each application date, in contrast to the other PECsw. For now, it is assumed that the pesticides travel to the catchment outlet with sufficient velocity, so that a superposition of breakthrough curves resulting from two subsequent applications is not necessary. However, this assumption might have to be revised.

PECsw due to drainage inputs

$$PECsw,drain\_m = Lsw,drain\_m_{catch} / (Baseflow + Drainflow\_m_{catch}) * GF \quad \text{(eq. 4.46)}$$

PECsw,drain_m	maximum daily concentration of the a.i. in surface water resulting from drainage inputs at the catchment outlet in month m (m = 1-240) [mg m^{-3} = µg L^{-1}]
$Lsw,drain\_m_{catch}$	maximum daily total drainage input of the a.i. into surface water in the catchment in month m (m = 1-240) [mg d^{-1}]
Baseflow	calendar-month-specific mean daily baseflow from area of interest at the catchment outlet [m^3 d^{-1}]
$Drainflow\_m_{catch}$	total daily drainflow volume entering the surface water network in the catchment on the day of the maximum daily pesticide drainage input in a month [m^3 d^{-1}]

PECsw due to surface runoff, erosion and lateral subsurface flow inputs

The reasoning for calculating a combined PEC for runoff/erosion and interflow is that in some soil types, surface runoff and erosion events usually also cause lateral subsurface flow.

$$PECsw,runoff/erosion/interflow\_m = (Lsw,runoff\_m_{catch} + Lsw,erosion\_m_{catch} * ERF + Lsw,interflow\_m_{catch}) / (Baseflow + Runoff\_m_{catch} + Interflow\_m_{catch}) * GF \quad \text{(eq. 4.47)}$$

with

PECsw,runoff/erosion/interflow_m	maximum daily concentration of the a.i. in surface water resulting from surface runoff, erosion and lateral subsurface flow inputs at the catchment outlet in month m (m = 1-240) [mg m^{-3} = µg L^{-1}]
$Lsw,runoff\_m_{catch}$	maximum daily total runoff input of the a.i. into surface water in the catchment in month m (m = 1-240) [mg d^{-1}]
$Lsw,erosion\_m_{catch}$	maximum daily total erosion input of the a.i. into surface water in the catchment in month m (m = 1-240) [mg d^{-1}]
$Lsw,interflow\_m_{catch}$	maximum daily total interflow input of the a.i. into surface water in the catchment in month m (m = 1-240) [mg d^{-1}]

$Runoff\_m_{catch}$	total daily surface runoff volume entering the surface water network in the catchment on the day of the maximum daily pesticide runoff input in a month [m^3 d^{-1}]
$Interflow\_m_{catch}$	total daily interflow volume entering the surface water network in the catchment on the day of the maximum daily pesticide interflow input in a month [m^3 d^{-1}]
ERF	fraction of particle-bound pesticide inputs (i.e. pesticide erosion inputs) that is transported downstream from its point of entry. It must be accounted for here that not all pesticide erosion inputs will contribute to PECsw: Strongly sorbing pesticides will remain adsorbed to particles (and thus to the bed sediment, to which the eroded sediment yield is added) to a large extent. ERF is estimated with a simple approach assuming linear sorption and instantaneous sorption equilibrium between the flowing water body and the bed sediment and neglecting sediment pore water. Under these strongly simplifying assumptions, EF is obtained as

$$\mathrm{ERF} = \frac{d_{sw}}{d_{sw} + K_{oc} * OC * BD * d_{sed}} \qquad \text{(eq. 4.48)}$$

with

d_{sw} = depth of water body at the point of entry (approximated as area-weighted mean depth over catchment) [m]

K_{oc} = normalized linear adsorption coefficient of the compound [L kg^{-1}]

OC = organic carbon content of sediment [-]; default: 0.05

BD = bulk density of sediment [kg L^{-1}]; default: 0.8

d_{sed} = depth of bed sediment at the point of entry [m]; default: 0.05

PECsw due to drainage and lateral subsurface flow inputs

Apart from the three PECsw equations given above, two further options for PECsw calculation are offered to the user. The first one is a combined PEC for drainage and interflow inputs. The reasoning is that the same rainfall events that cause drainflow in artificially drained soils are also likely to cause lateral subsurface flow in undrained soils susceptible to this process. Hence, drainage inputs and lateral subsurface flow inputs into surface water would coincide.

PECsw,drain/interflow_m = (Lsw,drain_m_{catch} + Lsw,interflow_m_{catch}) / (Baseflow + Drainflow_m_{catch} + Interflow_m_{catch}) * GF

PECsw due to drainage, surface runoff, erosion and lateral subsurface flow inputs

Since pesticide inputs via lateral subsurface flow can be coupled to both pesticide drainage inputs and pesticide surface runoff and erosion inputs, it can also occur that the maximum daily inputs in a particular month (1-240) via each of these pathways coincide on the same day.

PECsw,drain/runoff/erosion/interflow_m = (Lsw,drain_m_{catch} + Lsw,runoff_m_{catch} + Lsw,erosion_m_{catch} * ERF + Lsw,interflow_m_{catch}) / (Baseflow + Drainflow_m_{catch} + Runoff_m_{catch} + Interflow_m_{catch}) * GF (eq. 4.49)

4.7.2 Calculation of temporal CDF for PECsw,drift at the catchment outlet

The PECsw calculation is repeated for all application dates specified. Subsequently, the PECsw (variable numbers) at the catchment outlet are ranked and a cumulative relative frequency F is assigned to each of them by

F = rank / N (eq. 4.50)

with N being the total number of application dates, i.e. drift input events (different applications on the same day count as one event). The CDF can now be plotted, and its statistical population is the total number of drift input events per year.

Since the application dates don't follow a statistical distribution, but are specified by the user, it doesn't make sense to calculate a return period here.

4.7.3 Calculation of temporal CDF for the other PECsw

The PECsw calculation is repeated for all 240 months of the 20-year time series. Subsequently, the 240 PECsw at the catchment outlet are ranked and a cumulative relative frequency is assigned to each of them by

F = rank / (N + 1) = rank / (240 + 1) (eq. 4.51)

with N being the total number of monthly maximum daily pesticide inputs = 240. The cumulative relative frequency F in turn is inversely related to the return period T by T = 1 / (1

– F). Finally, the return period for a given monthly maximum concentration in surface water (e.g. 0.1 µg L-1) can be obtained by interpolation.

4.7.4 Calculation of the Gustafson factor

This section gives a brief description on how the Gustafson factor is obtained. The Gustafson equation (Gustafson et al., 2004, supporting information) is an analytical solution to the 1-dimensional Convection-Dispersion Equation (CDE) using the assumption that the dispersion coefficient increases linearly with the mean distance travelled. It has originally been derived to describe dispersion of pesticide plumes while leaching through field soils (Gustafson, 1988). However, it can also be used for describing geomorphological dispersion (i.e. dispersion caused by different flow path lengths and travel times from the various points of entry into the surface water network to the catchment outlet) in river networks (Gustafson et al., 2004). The equation basically converts a pulse input (e.g. a fictitious initial pesticide concentration given by total daily input / discharge) into a breakthrough curve at the catchment outlet (cf section 4.7.1). The factor GF is given as

$$\mathrm{GF} = \mathrm{R} * \frac{\exp(-(z - vt)^2 / 2kv_w vt^2)}{\sqrt{0.5\pi k v_w v t^2}} \qquad \text{(eq. 4.52)}$$

where

R	Normalization factor [-] required to properly scale the predicted breakthrough curve, because the analytical solution is for a Dirac pulse rather than a daily average input. The constant error function term in eq. 11 in Gustafson (1988) is also embedded in this factor. Gustafson et al. (2004, supporting information) recommend a value of R = 50.
z	mean stream length above catchment outlet [km]; is directly calculated in the GIS using the surface water network map. Since pesticides do not enter a catchment only at the stream origin (i.e. the spring), but potentially all over the catchment, it may be more appropriate to calculate z as "mean distance to the catchment outlet" (which would average distance to the catchment outlet over all points in the river network) rather than "mean stream length" (which would average distance to the catchment outlet only over the stream origins). However, which of both options is better will have to be determined in the evaluation exercise (WP6).

v	mean velocity of the transported solute (equal to v_w if there is no in-stream retardation, which we assume in FOOT-CRS) [km d^{-1}]
t	time since initiation of the pesticide input event
k	dimensionless constant describing the growth of the longitudinal dispersion coefficient ($D_L = k\ vv_wt$). In accordance with Gustafson et al. (2004, supporting information), k is set to 0.57.
v_W	mean stream flow velocity [km d^{-1}]. Stream flow velocity can be calculated from discharge, width and depth of the water body; depth can in turn be estimated from width, discharge and channel slope (Pistocchi and Pennington, 2006). Water body width is finally obtained from combining the UNH-GRDC discharge map (Fekete et al., 2000) with a width-discharge relation derived by Pistocchi and Pennington (2006).

4.7.5 Calculation of discharge and baseflow at the catchment outlet

- Baseflow is computed for each polygon/STU combination from polygon-specific discharge (source: GRDC Composite Runoff Fields, Fekete et al., 2000) and the FST-specific baseflow index (BFI)
- As a consequence, we have discharge and baseflow (in mm/d) attached to each polygon/STU combination and for each calendar month.
- It's still to be clarified whether discharge and baseflow at catchment outlet [in $m^3\ d^{-1}$] can be calculated as area-weighted sums over the catchment area of discharge and baseflow, resp., or if a flow accumulation is needed as suggested by Pistocchi and Pennington (2006).

5 ASSESSMENT METHODOLOGY FOR POINT SOURCE INPUTS INTO SURFACE WATER AND GROUNDWATER

Point sources are an important input pathway for pesticides into water bodies. However, at the national/EU scale, data availability on point sources is low, and point sources have to be mitigated against at farm and catchment scale anyway. Hence, it was not deemed meaningful to include point source calculations into FOOT-NES, and point sources are only considered in FOOT-FS and FOOT-CRS.

The original proposed use of the model HARDSPEC (Hollis et al., 2004) turned out as not feasible, because the relatively complex HARDSPEC model requires too too many input data that the user usually doesn't have available. Thus, a simpler, more pragmatic approach was pursued.

5.1.1 Point source inputs in FOOT-FS

Given the large uncertainties associated with the assessment of point source inputs into water bodies, for Foot-FS we have decided not to attempt calculations of point source inputs. Instead a separate audit/questionnaire was developed to remind the user what they should be doing to minimise point source releases.

Point Source Audit for Pesticides

Reference	Question (black) + explanation (blue)	Effectiveness Score	Cost Category
1,2,4,6,7,8,10,11,14,16,19,22,23,24	Is the site you use for pesticide activities (preparation, filling, equipment washing, loading etc.) purpose built and state-of-the art? Examples include: the use of biobeds / permeable surfaces where drained liquids are collected and safely disposed of / bunded & contained areas / steel grid system. Never use soak-aways.	High (70-50%)	Low
1,2,4,6,7,8,10,11,14,16,19,22,23,24	Do you avoid carrying out pesticide activities (preparation, filling, equipment washing, loading etc.) on porous surfaces such as concrete and surfaces that drain directly into to ditches or watercourses? Whilst porous / permeable surfaces can cause pesticide to drain away into the environment (unless they are contained and fluids collected) non permeable surfaces can encourage run-off.	High (70-50%)	Low
1,2,4,6,7,8,10,11,14,16,19,22,23,24	Is the site used for pesticide activities at least 30 m away from water boreholes, wells and watercourses or do you fill/wash in the field where spraying is to take place?	High (~50%)	Low - moderate
7,14,19,24	Do you avoid the occurrence of back-siphoning into the water system when using supply hoses for filling or washing etc.? The sudden loss of pressure can allow dirty water to be sucked into the supply pipes, which would contaminate the water system, anti-backflow systems & vacuum breakers	Moderate	Low
11	Do you transport pesticides around the farm in sealed, locked containers?	Low	Low
22	Do you have written plans for emergency procedures to deal with spills and operator contamination?	Moderate	Low
1,5,6,8,9, 11,15,16,20,22, 23,24,25	Do you carry out regular maintenance inspections of sprayer equipment? Equipment should be regularly checked for leaks and malfunctions, repairs should be carried out promptly. Equipment must be fit-for-purpose.	High (~70%)	Variable

Table 9. General good practice

Reference	Question	Effectiveness Score	Cost Category
8,16	Do you store your sprayer under cover to avoid rain splash?	Low	Variable
11,14,26,28	Do you have dedicated, purpose built pesticide storage facilities? For small quantities this should be a lockable, fire-resistant, frost-proof, spill proof container. For larger quantities the storage facility should be lockable, bunded, frost-proof, fire-resistant with an impermeable base and spill controlled.	Moderate	Moderate-high

Table 10. The pesticide store

Reference	Question Y/N	Effectiveness Score	Cost Category
3,7,9,16,19,22, 24,25	Do you, wherever possible, use systems especially packaged to reduce the risk of pesticide losses and spills? For example the use of closed transfer systems, direct transfer systems, induction hoppers and anti-glug necks?	High	Moderate
7,9,11,14,15,16,22,28	When filling, do you ensure that you are well prepared to handle any spills – small splashes and major spills – quickly and effectively? This should include having containment equipment, absorbent materials buckets and shovels at hand. Never wash down contaminated areas.	High	Moderate

Table 11. Preparation – filling and mixing

Reference	Question	Effectiveness Score	Cost Category
6,7,11,15, 22,25	Do you clean the sprayer and other equipment in the field being sprayed? This should include washing sprayer body and washing contaminated mud from wheels	Moderate	
1,7,14,23,27	Do you further dilute left-over spray and apply to crop taking care not to exceed the maximum crop dose?	Moderate	Low
14,24	Do you make effort to minimise waste in all areas of pesticide use? This should include: careful assessment of volumes required, careful stock management, use of returnable packaging or minimal packaging systems (closed-transfer, soluble packs, direct injection etc).	Low	Moderate
11,14	Do you have a dedicated storage area which is under cover and bunded for waste containers? Empty waste containers should not be stored outside.	Moderate	Low - Moderate
7,9,14,19,23	Do you pressure wash or triple rinse containers – unless the label advises otherwise?	Moderate	Low
14	Do you crush or make holes in used containers? Used containers must never be reused. Crushing or piercing ensures reuse is not possible.	Moderate (~20%)	Low
8,9,15,20,22	Unless crushed, do you store waste containers upright and lidded. Containers must not be inverted and allowed to drain after washing.	Moderate	Low
1,8,9,14,15, 20,22,24,27	Do you ensure safe disposal of all pesticides, their packaging and handling equipment? This must include use of registered disposal companies, gloves should be placed inside cardboard packaging, foil seals and lids must also be placed inside card packaging or container.	Moderate (~20%)	Moderate

Table 12. Waste management

References

Name	Published by	Language	Country	Usefulness
Environmentally sensitive farming powerpoint	ADAS/Defra	English	UK	Useful
Environmentally sensitive farming powerpoint	ADAS/Defra	English	UK	Moderate
Application technology	Pesticide Forum	English	UK	Some
Pesticides in water	PAN UK	English	UK	Some
EU Policy for sustainable use of pesticides	EC	English	EU	Some
Annual Report	Pesticide Forum	English	UK	Some
Topps Point source pollution audit	Topps/Life	Danish	EU	Useful
ECPA Water Quality Initiatives	ECPA	English	EU	Some
VI Keep water clean card	VI	English	UK	Not much
The VI & water pollution	Friends of the Earth	English	UK	Not much
CCPM 2007	VI	English	UK	Moderate
H2OK Water Catchment Protection	VI	English	UK	None
Keeping raw water resources safe from pesticides	EU	English	EU	Not much
COGAP – Water	UK	English	UK	Useful
River Cherwell Catchment study	UK	English	UK	Some
How pesticides get into water…. (Pesticide Outlook)	UK Andre Carter	English	UK	Useful
Corpen report	Ministere de L'amenagement du Territoire et de L'environnement	French	France	Some
Reducing point source pollution	CleanRegion	English	UK	Useful
Cleaning sprayer equipment	Univ. Missouri Extension Agenc	English	USA	Some
Use of models…. (Pest Management Science)	SCI J. Garratt	English	UK	Moderate
Reichenberger et al. (2007) (based on FOOTPRINT DL7)	The FOOTPRINT team	English	Germany	
Protecting water… (Pesticide Outlook)	S. Higginbotham	English	UK	Useful
Risk of water contamination by PPP… (Ag Eng)	P. Jaeken	English	Belgium	Moderate
Arvalis presentation	Arvalis	English	French	Not much
TIBRE – Crop Protection technologies	SNH	English	UK	Some
Guidance on storing pesticides	HSE	English	UK	Not much
Disposing of pesticide waste	Defra	English	UK	Moderate
Pesticide 'Green' code of practice	Defra	English	UK	Moderate

5.1.2 Point source inputs in FOOT-CRS

In FOOT-CRS we have decided to keep the assessment of releases to waters from point sources separate from the modelling of diffuse inputs, since it is not possible to undertake modelling of point source inputs with an accuracy comparable to modelling of diffuse inputs. Nevertheless, despite the large uncertainties and lack of available input data associated with point source assessments, the FOOT-CRS user will need to have an idea about the contribution of point sources to groundwater and surface water contamination in the catchment of interest. For this reason, we propose a set of simple calculations which rely exclusively on user input (since it's practically impossible to give any default values).

User input in the "pesticide scenario manager" module for the FOOT-CRS point source assessment:

(This is optional input. It's needed only for point source assessment, and the user is free to perform a point source assessment or not. The user may also enter part of the requested input, i.e. fill in only one or more subsections and leave the others blank.)

I. filling/cleaning (only field application month)

1. number of farms in the catchment N_f
2. number of field sprayers in the catchment N_s
3. pesticide mass in one field sprayer tank filling m_{tank}
4. expected number of filling or cleaning operations per farm N_{fcf}
5. expected number of filling or cleaning operations per field sprayer N_{fcs}
6. expected % loss of pesticide mass in one tank filling due to a regular filling or cleaning operation related to the application of concern $\%loss_{fc}$

II. accidental spills (field and farmyard application months)

7. expected number of accidental spills per farm N_{sp}
8. expected % loss of pesticide mass in one tank filling due to accidental spills etc. $\%loss_{sp}$

III. leakages: (all year)

9. expected number of leakages from full or empty containers in the catchment N_l
10. expected monthly mass loss due to leakages in the catchment m_{lk} (g d^{-1})
11. expected fraction of mass leaked leaching to gw $\%_{lkgw}$
12. expected fraction of mass leaked contributing to surface water contamination $\%_{lksw}$

IV. intentional applications (only farmyard application months)

13. month(s) of farmyard application month fam

14. number of intentional applications on the farmyard in the respective fam N_{fd} (makes only sense for herbicides, of course)
15. expected pesticide mass applied to a farmyard in an intentional application in the respective fam m_{fd}

V. fate on farmyard:

16. dissipation half-life on farmyard surface $DT50_f$(d)
17. expected time period to next significant rainfall event (e.g. ≥ 5mm) after filling/cleaning operation or intentional application T_f (d)
18. expected number of significant rainfall events (e.g. ≥ 5mm) in month i N_p ($N_p \leq 30/T_f$)

Applied amounts

From the application rate, the agricultural statistics and the fraction of crop area that is treated we know the total amount of the pesticide that is sprayed in the catchment (m_{tot}).

Simplifying assumptions:

1. "Closed system"
   - no filling/cleaning operations from applying outside the catchment;
   - no applications in catchment with filling/cleaning operations performed outside the catchment
2. cleaning occurs in the same month as application
3. leakages behave as continuous sources
4. no sorption on the farmyard
5. complete connectivity is given to the surface water body (either via hard surfaces or the sewer system)
6. no dissipation during transport
7. farmyards are not flushed by the farmer, but are exclusively rinsed by rain.
8. Losses due to leaking sprayers during driving to or returning from fields are counted as farmyard losses, i.e. roads are treated in the same way as farmyards

(4.-6. are clearly worst-case assumptions)

Calculations

1. Calculate monthly load onto all farmyards in the catchment due to agricultural applications m_{tfag} (in the month of ag. application)

Two options for the user:

- $m_{tfag} = N_f * N_{fcf} * m_{tank} * \%loss_{fc}$
- $m_{tfag} = N_s * N_{fcs} * m_{tank} * \%loss_{fc}$

2. calculate total load onto all farmyards in the catchment due to direct farmyard applications m_{tfd} (in the respective fam)
   $m_{tfd} = N_{fd} * m_{fd}$

3. calculate monthly input into gw due to leakage in catchment
   $m_{lkgw} = m_{lk} * \%_{lkgw}$

4. calculate monthly input into sw due to leakage in catchment
   $m_{lksw} = m_{lk} * \%_{lksw}$

5. calculate monthly load onto all farmyards in the catchment due to accidental spills m_{tfsp} (in the month of ag. application and the fam's)
   $m_{tfsp} = N_f * N_{sp} * m_{tank} * \%loss_{sp}$

6. Total load onto all farmyards in the catchment in a given month i $m_{tf,i}$
   $m_{tf,i} = m_{tfag,i} + m_{tfd,i} + m_{tfsp,i}$ (not all summands occur in all months)

7. Total input into surface water from farmyards in the catchment in a given month i $m_{tfsw,i}$
   $m_{tfsw,i} = m_{tf,i} * \exp(-\ln 2 * T_f/DT50_f)$

8. Max. daily input of pesticides into surface water from farmyards in the catchment in a given month i $m_{tfsw,id}$
   $m_{tfsw,id} = m_{tfsw,i} / N_p$

9. PECsw due to input of pesticides from farmyards and leakage in a given month i $PECsw_{,pi}$:
   $PECsw_{,pi} = (m_{lksw}/30 + m_{tfsw,id}) / Q(t) * GF$

where

Q(t) daily river discharge from area of interest [m³] (available as monthly means)

GF Peak Concentration Reduction Factor from Gustafson equation (CDE analogon). The Gustafson equation converts a pulse input into a breakthrough curve at the catchment outlet → the peak concentration at the outlet will be lower than “input / discharge”.

Accounting for mitigation of point source inputs:

This must be done in the Mitigation Manager, which is included in the Pesticide Scenario Manager module:

1. mixing pesticides, filling and cleaning sprayers on biobeds → user enters percentage of farms / sprayers (depending on the option chosen for m_{tfag} calculation) where filling and cleaning are performed on a biobed or on the field → reduce m_{tfag} by this percentage
2. safe storage and disposal of containers → user enters percentage of farms where empty and full containers are stored safely → reduce m_{lk} by this percentage
3. no application on the farmyard → user enters percentage of reduction of applications on the farmyard in the catchment → reduce m_{tfd} by this percentage
4. sharing spraying equipment or spraying by contractors? → user enters percentage by which filling/cleaning operations are reduced → reduce m_{tfag} by this percentage → user can also change $\%loss_{fc}$ (to account more more or less careful handling of spraying equipment and pesticides)

1.-3. mainly reflect the success of information/awareness campaigns.

Regular inspection of sprayers should be a matter of course. At the moment, it cannot be accounted for quantitatively. It is therefore suggested to just highlight the message that regular inspection is important and that the degree of sprayer inspection (or the state of sprayers in use in the catchment) should be considered when entering $\%loss_{fc}$, since losses on roads are counted as losses on farmyards in this simplified assessment.

6 INCORPORATING THE EFFECT OF MITIGATION MEASURES

The following mitigation measures will be available as options for the user to reduce pesticide inputs into surface water and groundwater.

List of mitigation measures explicitly or implicitly included in the different tools

mitigation measures

measures are already implicitly or explicitly included in Pesticide Scenario Manager (FOOT-CRS/-NES) / Pesticide Programme Manager + Scenario Builder (FOOT-FS)
effect is directly calculated in the GIS (if spatial resolution of input maps is fine enough)
effect is directly calculated in the GIS, but a buffer has to be specified by the user beforehand
reflected in the Mitigation Manager as spatially variable mitigation factor
reflected in the Mitigation Manager as spatially constant (global) mitigation factor
reflected in the FOOT-FS Scenario Builder
reflected in the My Equipment section of FOOT-FS
included explicitly or implicitly n the FOOT-CRS point source assessment (part of the FOOT-CRS Pesticide Scenario Manager)
not considered at this stage (possibly in later versions)

pathway	FOOT-FS	FOOT-CRS	FOOT-NES
drift	1. reduction of application rate 2. product substitution) 3. minimum distances 4. riparian buffer strips and hedges 5. change crop / land use 6. drift reducing technology (several options) 7. change of application date (matters only for pome/stone fruit)	1. reduction of application rate 2. product substitution 3. minimum distances 4. riparian buffer strips and hedges 5. change crop / land use 6. drift reducing technology (several options) 7. change of application date (matters only for pome/stone fruit)	1. reduction of application rate 2. product substitution 3. minimum distances 4. riparian buffer strips and hedges 5. change crop / land use 6. drift reducing technology (several options) 7. change of application date (matters only for pome/stone fruit)
drainage	1. reduction of application rate 2. product substitution 3. shift of application date? (only monthly shifts lead to a change in results) 4. application restrictions in time and/or space 5. change crop / land use	1. reduction of application rate 2. product substitution 3. shift of application date? (only monthly shifts lead to a change in results) 4. application restrictions in time and/or space 5. change crop / land use	1. reduction of application rate 2. product substitution 3. shift of application date (only monthly shifts lead to a change in results) 4. application restrictions in time and/or space 5. change crop / land use
leaching	1. reduction of application rate 2. product substitution 3. shift of application date (only monthly shifts lead to a change in results) 4. application restrictions in time and/or space 5. change crop / land use	1. reduction of application rate 2. product substitution 3. shift of application date (only monthly shifts lead to a change in results) 4. application restrictions in time and/or space 5. change crop / land use	1. reduction of application rate 2. product substitution? 3. shift of application date (only monthly shifts lead to a change in results) 4. application restrictions in time and/or space 5. change crop / land use
Surface runoff and erosion	1. reduction of application rate 2. grassed edge-of-field buffer strips 3. product substitution 4. riparian buffer strips and hedges 5. shift of application date (only monthly shifts lead to a change in results) 6. application restrictions in time and/or space	1. reduction of application rate 2. grassed edge-of-field buffer strips 3. product substitution 4. riparian buffer strips and hedges 5. shift of application date (only monthly shifts lead to a change in results) 6. application restrictions in time and/or space	1. reduction of application rate 2. grassed edge-of-field buffer strips 3. product substitution 4. riparian buffer strips and hedges 5. shift of application date (only monthly shifts lead to a change in results) 6. application restrictions in time and/or space

	7. change crop / land use 8. grassed waterways 9. constructed wetlands	7. change crop / land use 8. grassed waterways (this is basically a grassed buffer strip in slope direction, usually located where overland flow accumulates (little talwegs on a slope); it's NOT a ditch or other water body) 9. constructed wetlands 10. strip cropping	7. change crop / land use 8. grassed waterways 9. constructed wetlands
Point sources	No calculations, instead FOOT-FS point source audit (cf. section 5.1)	1. mixing pesticides, filling and cleaning sprayers on biobeds or on the field 2. safe storage and disposal of containers 3. no application on the farmyard? 4. Characteristics of farmyards in the catchment (paved, asphalt, dirt, concrete)? 5. Degree of connectedness of farmyards in the catchment to sewer system? 6. sharing spraying equipment or spraying by contractors? 7. regular inspection of sprayers	not applicable

Table 13. List of mitigation measures included in the different tools

7 CONCLUSIONS

The approaches to calculate pesticide losses from fields, pesticide inputs into water bodies and resulting concentrations as well as spatial aggregation procedures have been described in detail for each of the three tools. It may occur that during the later stages of the programming or during the evaluation phase changes to some methodologies become necessary. This document therefore only reflects the current state of knowledge and development. The document forms the basis of the technical reports of FOOT-NES and FOOT-CRS, and parts of it will also be included in the technical report of FOOT-FS. The technical reports will of course include all changes that may become necessary in the future development.

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