

Technical Report

CONTINUOUS-SIMULATION COMPONENTS FOR PESTICIDE ENVIRONMENTAL ASSESSMENTS WITH VFSSMOD: 2. VFS PESTICIDE RESIDUE BETWEEN RUNOFF EVENTS

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Executive Summary

VFSMOD (Muñoz-Carpena et al., 1999; 2004) is a numerical, storm-based design model. During the rainfall-runoff event it calculates the dynamic hydrological and transport processes occurring in the vegetative filter strip (VFS). For this it uses initial conditions (soil, water, vegetation) and boundary conditions (rainfall, inflow runoff from the field) and calculates outflow hydrographs and pollutographs (sediment, pesticides, reactive solutes) for the storm, as well as the water and mass balances at the end of the storm. The model has been coupled for use into current long-term higher-tier pesticide environmental assessment framework (US EPA and EU FOCUS surface water) where flow, sediment and pesticide runoff at the end of the field is calculated by the model PRZM, and VFSMOD routes it from the field through a VFS of desired characteristics to estimate potential load reductions before entering the aquatic environment. Long-term simulations require realistic initial conditions at the beginning of each runoff event in the time series (initial soil water, pesticide residue and vegetation status).

Herein, we present a simplified VFSMOD pesticide mass balance component to estimate surface pesticide residue in the buffer at the end of a runoff event and its degradation towards the next runoff event in the times series.

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Simplified VFSMOD Pesticide Mass Balance and Long-Term Surface Soil Water Dynamics for Interface with the Continuous EPA/FOCUS Simulation Framework

Description

VFSMOD (Muñoz-Carpena et al., 1999; 2004) is a numerical, storm-based design model. During the rainfall-runoff event it calculates the dynamic hydrological and transport processes occurring in the vegetative filter strip (VFS). For this it uses initial conditions (soil water, vegetation) and boundary conditions (rainfall, inflow runoff from the field) and calculates outflow hydrographs and pollutographs (sediment, pesticides, other) for the storm, as well as the water and mass balance at the end of the storm (Fig. 1). The model can be coupled within current high-tier environmental assessment frameworks (US EPA and EU FOCUS surface water), where the water, sediment and pesticide runoff at the end of the field is calculated by the model PRZM, and VFSMOD routes it from the field through a VFS of desired characteristics to estimate potential load reductions before entering the aquatic environment described by EXAMS (US-EPA) or TOXWA (EU-FOCUS) models.

Long-term simulations require realistic initial conditions (initial soil water, pesticide residue, vegetation status) in the VFS at the beginning of the calculations for each runoff event in the time series. Herein, a simplified VFSMOD pesticide mass balance and degradation component is proposed to estimate surface pesticide residue for buffer efficiency calculations.

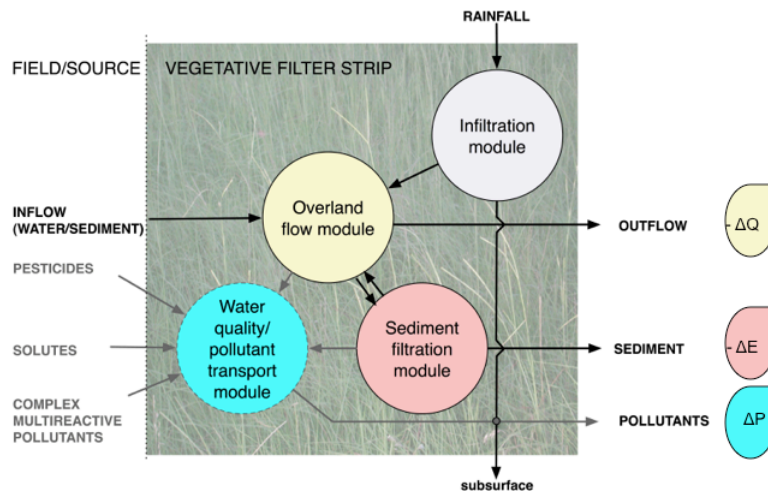


Figure 1. VFSMOD dynamic flow and sediment

The new VFSMOD component is based on simplified calculations of pesticide mass balance and degradation on the surface of the VFS, performed after the simulation of pesticide trapping and transport through the filter. The pesticide residue is determined from the water, sediment and pesticide mass balance components calculated by VFSMOD at the end of the runoff event. The residual pesticide in solid phase is estimated as pesticide bonded to the sediment trapped in the filter during the event. A fraction of the dissolved phase pesticide trapped (moved to the subsurface through infiltration), that on the thin soil mixing layer, is considered for degradation towards the next runoff event in time (Figure 2).

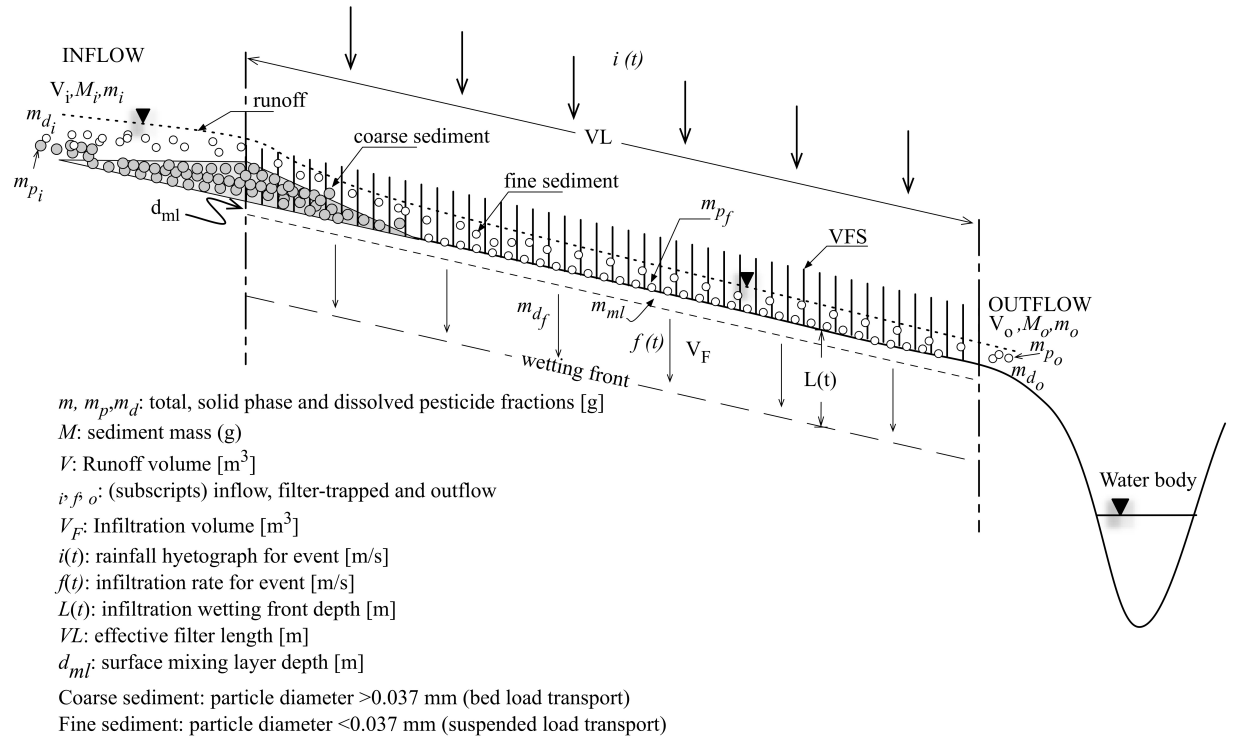


Figure 2. Proposed conceptual pesticide mass balance

Residual pesticide after the event, i.e. attached to runoff sediment trapped on the filter and on the mixing layer, is handled as a worst-case scenario where all mass is available for degradation and transport (and trapping) towards the next event. The total surface pesticide mass retained in the filter at the end of the event is degraded with daily time increments based on soil temperature and water conditions until the next runoff event in the series provided by PRZM.

The assumptions, inputs and the calculation procedure are described below along with an application example, and the new VFSMOD component developed for these calculations (Appendices).

Pesticide partitioning and residue

In the EU and USA higher-tier assessments rely on the model PRZM for estimation of water, sediment and pesticide mass leaving the agricultural field (or similar source area). This provides total incoming mass (water, sediment and pesticide) into the filter. If linear sorption equilibrium between solid and dissolved pesticide phases is assumed, the pesticide can be partitioned using the distribution coefficient value K_d for the particular pesticide,

$$K_d = \frac{S}{C} = \frac{m_p/M_s}{m_d/V_w} \quad [\text{L}^3\text{M}^{-1}] \quad (1)$$

where S [$\text{M}\cdot\text{M}^{-1}$] is pesticide adsorbed to the sediment/soil, C [$\text{M}\cdot\text{L}^{-3}$] is the dissolved pesticide concentration, m_p, m_d [M] are mass of pesticide in solid (sorbed to particulates) and liquid phases, M_s [M] is the mass of the solid phase and V_w [L^3], the volume of the liquid phase

(runoff). Notice also that K_d is related to the organic carbon sorption coefficient K_{oc} , that is more commonly available for pesticides, and the soil percentage organic carbon (OC(%)) as,

$$K_d = \frac{K_{oc} * OC(\%)}{100} \quad [L^3M^{-1}] \quad (2)$$

For each event dissolved pesticide and the component sorbed to eroded soil/sediment trapped in the filter is calculated using the linear equilibrium assumptions (K_d) based on PRZM inputs (incoming pesticide mass, m_i , sediment mass M_i , and runoff inflow, V_i) and VFSSMOD outputs (sediment trapped and out, M_i and M_o , runoff outflow, V_o) and soil mixing layer characteristics (depth d_{ml} [L], saturated water content θ_s [-] and bulk density ρ_b [M.L⁻³]) (Fig. 2).

The residual pesticide in the surface of the filter after the event is calculated as the mass of the pesticide deposited with the sediment during the event (solid phase), plus the amount contained in the mixing layer based on linear equilibrium distribution during the event (Fig. 3).

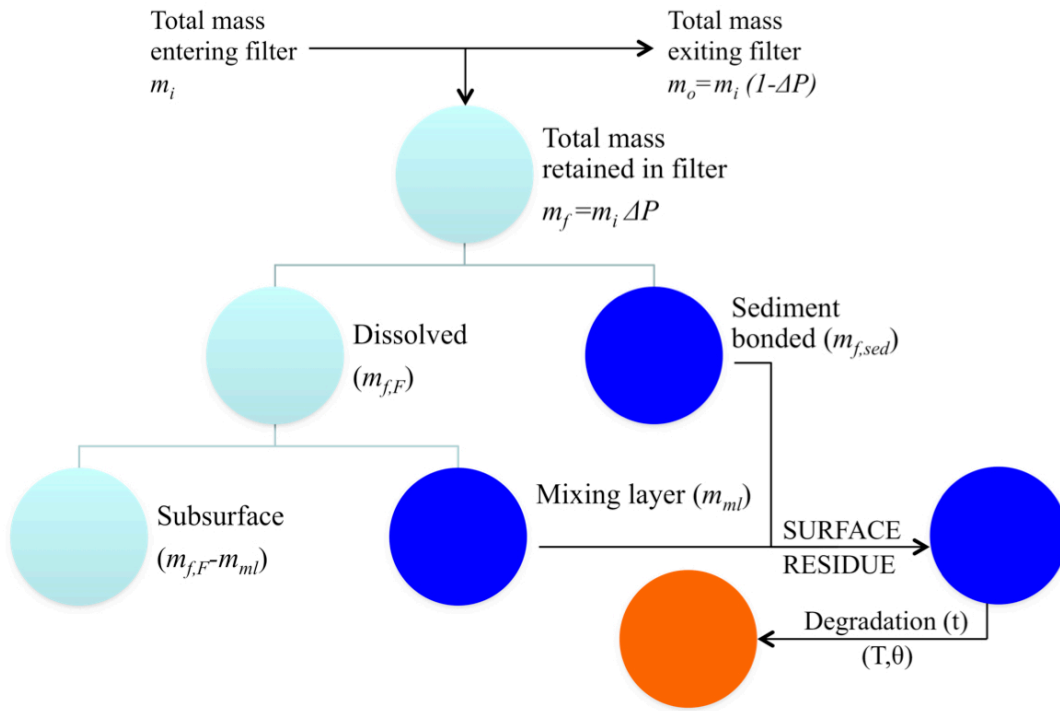


Figure 3. Partitioning of pesticide retained in VFS for degradation calculations.

A central assumption of the calculations proposed is that for the short-duration of a typical runoff event (minutes to hours) the sediment solid phase pesticide concentration will not change during the event so that the incoming (S_i), filter-trapped (S_f) and outgoing (S_o) solid phase concentrations are the same,

$$S_i \approx S_f \approx S_o \quad (3)$$

The partition of the incoming pesticide mass (m_i) can be estimated assuming perfect mixing of total mass of sediment pesticide and inflow, and linear adsorption equilibrium between the liquid or dissolved (m_{d_i}) and solid or particulated (m_{p_i}) phases,

$$m_i = m_{p_i} + m_{d_i} \Rightarrow m_{d_i} = m_i - m_{p_i} \quad (4)$$

$$K_d = \frac{S_i}{C_i} = \frac{m_{p_i}/M_i}{m_{d_i}/V_i} \Rightarrow m_{p_i} = \frac{m_i M_i K_d}{V_i + M_i K_d} \Rightarrow S_i = \frac{m_{p_i}}{M_i} = \frac{m_i K_d}{V_i + M_i K_d} \quad (5)$$

For the mass balance within the filter at the end of the event, the pesticide mass trapped in the filter (m_f) can be calculated as the difference between in/out masses, and this as the sum between the mass adsorbed to the sediment deposited in the filter ($m_{f, sed}$) and the dissolved mass infiltrated in the soil during the event ($m_{f, F}$) (Fig. 3),

$$m_f = m_i - m_o = m_i \Delta P = m_{f, sed} + m_{f, F} \quad (6)$$

where ΔP is the filter trapping efficiency of pesticide mass (calculated by VFSSMOD for each event). The sediment-adsorbed fraction deposited on the VFS surface during the event can be estimated proportional to the sediment mass deposited in the filter,

$$m_{f, sed} \approx S_i (M_i - M_o) \Rightarrow m_{f, F} = m_f - m_{f, sed} = m_i \Delta P - S_i (M_i - M_o) \quad (7)$$

The pesticide mass contained in the mixing layer can be calculated as the total mass in equilibrium within the mixing layer soil volume ($V_{ml} = d_{ml} \times VL \times b$, see Fig.1). The depth of the mixing layer is recommended to be $d_{ml} = 2$ cm for consistency with that used in PRZM. The new module also allows the user to modify this as needed based on other values reported in the literature (typically 0.5-5 cm). The dimension perpendicular to the flow direction through the filter ($b = \text{FWIDTH}$) is set to $b = 1$ m, i.e. per unit of filter width.

It is assumed that the runoff solution has saturated the soil runoff mixing layer, i.e. that the soil water content is at saturation (θ_s) and that the pore water concentration is equal to that of the average pesticide concentration of the water retained in the filter during the event (C_F). Although at the beginning of the event the concentration of the soil pore water (C_{pw}) will likely be lower than that on the surface (C_F), infiltration during the event will continuously flush the porewater, eventually approaching the concentration at the surface. The assumption that the infiltration concentration equals that of the pore water is likely to result in slightly higher calculated values in the pore water than those in the field, so this represents a conservative assumption in terms of residual mass in the filter. The average dissolved phase concentration of the water retained in the filter during the event is estimated as,

$$C_F = \frac{m_{f, F}}{V_F} \approx C_{pw} \quad \text{and} \quad (8)$$

$$V_F = (V_i + V_R) - V_o \quad (9)$$

Where V_F and V_o are the volumes of water retained in the filter and exiting as runoff, respectively, calculated in VFSSMOD, V_R is the rainfall volume for the event. Thus, the pesticide trapped in the mixing layer (m_{ml}) is estimated as the sum of the porewater ($m_{ml, d}$) and solid phase ($m_{ml, p}$) masses,

$$m_{ml} = m_{ml, d} + m_{ml, p} \approx (\theta_s C_F + \rho_b S) V_{ml} = (\theta_s + K_d \rho_b) C_F d_{ml} \cdot b \cdot VL \quad (10)$$

Note that the mixing layer bulk density (ρ_b [M.L^{-3}]) can be estimated for mineral soils based on the top soil saturated water content (θ_s [-], an existing VFSSMOD input) by assuming the specific density of the soil $\rho_s = 2.65$ Kg/L and,

$$\theta_s \approx 1 - \frac{\rho_b}{\rho_s} \Rightarrow \rho_b \approx (1 - \theta_s) \rho_s \quad (11)$$

Finally, the total mass of pesticide in the surface considered in the degradation calculations between events is the sum of the pesticide adsorbed to the sediment trapped during the event and the pesticide (solid and liquid phases) contained in the mixing layer,

$$m_{res} = m_{f, sed} + m_{ml} \quad (12)$$

Residual pesticide degradation between events

The dissolved pesticide in the mixing layer arising from the infiltration component is considered part of the surface residual mass for pesticide degradation calculations. Thus, the residual pesticide in the filter (m_{res}) is lumped into single mass component (mixing layer + adsorbed sediment trapped on surface) and degraded as a function of time (first order decay), where k (day) is the pesticide degradation rate,

$$\frac{dm_{res}}{dt} = -k \cdot m_{res} \Rightarrow m_{res}|_{t_1} = m_{res}|_{t_0} e^{-kt} \quad (13)$$

To accommodate different regulatory environments, four types of k degradation rates are included (controlled by the input flag IDG in the IWQ file, Table 1). Generally, the degradation rate can be expressed as the product of the reference rate (k_{ref}) and modifiers to incorporate the effects of temperature (k_T) and moisture (k_θ),

$$k = k_{ref} * k_T * k_\theta \quad (14)$$

Table 1. Pesticide degradation rate formulations included in the model.

IDG	Type	k_{ref}	k_T	k_θ	T_{ref}, E_a
1	EU-FOCUS (1996 rev. 2006; EFSA Opinion, 2008)	k_{ref}	$e^{\frac{E_a}{R} \left(\frac{1}{T_{ref}} - \frac{1}{T} \right)}$	$\left(\frac{\theta}{\theta_{ref}} \right)^{-\beta}$	293.15 K 65.4 kJ/mol ($Q_{10}=2.58$)
2	US-EPA	k_{ref}	1	1	298.15 K --
3	$k = k(T)$	k_{ref}	$e^{\frac{E_a}{R} \left(\frac{1}{T_{ref}} - \frac{1}{T} \right)}$	1	298.15 K 49.5 kJ/mol ($Q_{10}=2$)
4	$k = k(\theta)$	k_{ref}	1	$\left(\frac{\theta}{\theta_{ref}} \right)^{-\beta}$	298.15 K --

where m_{res} : residual pesticide in the filter; t = time (days); T = average daily surface soil temperature (K) between events; θ = average daily surface soil moisture between events [$m^3 m^{-3}$]; $k=k(T, \theta)$ =pesticide degradation rate adjusted for (T, θ) (day^{-1}); k_{ref} = pesticide degradation rate (day^{-1}) at standard conditions of $T(T_{ref})$ and $\theta(\theta_{ref} = \theta_{FC}$ =field capacity) (**note**: k_{ref} is related to the pesticide half-life ($t_{1/2}$, day) by $k_{ref} = \ln(2)/t_{1/2}$); E_a = degradation activation energy (10-90 kJ/mol); R = gas constant, 8.314×10^{-3} kJ/mol/K; β = constant (recommended 0.7, FOCUS v2.0, 2006).

The calculations are carried out on a daily time step between each event. Soil temperature is needed on the top soil mixing layer ($d_{ml} = 2$ cm based on PRZM). Based on the heat transport

equation, the air temperature attenuates and delays in time through the soil profile until reaching a constant temperature deeper in the profile. Thus, a reasonable approximation for a thin surface layer on the top of the soil is $T_{top} \approx T_{air}$. Soil moisture (θ) is estimated based on FAO-56 crop water stress-adjusted method (FAO, 1998) with the program THETAFAO described in Report 1.

The residual pesticide mass at the beginning of the next event is considered as a worst-case scenario to be fully mixed with the incoming pesticide mass into the filter. For this, it is added to the incoming pesticide mass into the filter, and the pesticide trapping efficiency calculated for that event (ΔP) is applied to the sum to obtain the outflow total pesticide mass leaving the filter in runoff at the end of the event,

$$m'_i = m_i + m_{res}|_{t_{end}} \Rightarrow m_o = m'_i(1 - \Delta P) \quad (15)$$

Pesticide partitioning of the filter outflow

In order to link the pesticide outflow concentration from the VFS with aquatic models representing the water body adjacent to the field in current regulatory frameworks (EPA-EXAMS, EU-TOXWA) it is necessary to estimate the partitioning of the total sediment outflow mass from the filter into dissolved and particulated fractions. As before (eq. The partition of the outgoing pesticide mass (m_o) can be estimated assuming perfect mixing of total mass of sediment pesticide and outflow, and linear adsorption equilibrium between the liquid or dissolved (m_{do}) and solid or particulated (m_{po}) phases,

$$m_o = m_{p_o} + m_{d_o} \Rightarrow m_{d_o} = m_o - m_{p_o} \quad (16)$$

$$m_{p_o} = \frac{m_o M_o K_d}{V_o + M_o K_d} \quad (17)$$

Assumptions and limitations

Table 2 summarizes the main assumptions contained in the proposed new module.

Table 2. Main assumptions and operational constraints of the proposed pesticide degradation module

Component	Assumptions/Limitations
Pesticide mass balance	<ul style="list-style-type: none"> • Linear adsorption equilibrium • Saturation of sediment-adsorbed pesticide concentration ($S_i \approx S_f \approx S_o$), i.e. it does not change during short time event • Mixing zone with fixed depth, porewater concentration at the end of event equivalent to that of infiltrating water.
Pesticide degradation	<ul style="list-style-type: none"> • Soil mixing layer daily temperature considered equal to air temperature • Soil mixing layer daily moisture approximated as the average moisture for the root zone • Liquid and solid phase pesticide in mixing layer is lumped together with trapped sediment-bonded mass to calculate degradation • Activation energy for degradation and the moisture exponent values are valid for field conditions
Incoming pesticide (next event)	<ul style="list-style-type: none"> • All residual mass in mixing layer after degradation is added to new field incoming mass for next event in time series

New VFSMOD input requirements - Revised IWQ input file

Sources for the pesticide degradation module inputs are shown in Table 2. No new input factors other than those already available in the PRZM/VFSMOD SWAN framework are required to complete the calculations.

Table 3. New VFSMOD input requirements (IWQ file)

Input	Source	Comment
<i>IDG</i>	User	1-4, to select pesticide degradation rate formulation (Table 1)
<i>nday</i>	PRZM	No. days to next runoff event
T_j ($j=1, nday$)	FOCUS	Degradation equation
θ_j ($j=1, nday$)	THETAFAO/EU SWAN Shell	From MET file info: ETP, PRECIP, WIND, Tmax, Tmin
k_{ref}	PRZM	Degradation equation
<i>FC</i>	PRZM	Degradation equation
d_{mi}	Recommended in PRZM (2 cm)	Mass balance at the end of the event
m'_i	PRZM+ VFSMOD residue (degraded from previous event)	Runoff pesticide mass entering filter

Sample application

For illustration, an example of pesticide partitioning and degradation between events is presented. The case corresponds to a runoff event on day December 15, 1984 with an event following 3 days later. Water, sediment and pesticide runoff from a 1 ha (100x100 m) agricultural field is calculated by the PRZM model and transferred to VFSMOD to obtain the water, sediment and pesticide mass balance at the adjacent VFS of dimensions VL=5 m (distance to the water edge from the field) and FWIDTH=100 m. Inputs and outputs for the event, including residual pesticide in surface (sediment bonded + mixing layer) at the beginning of the next event are presented below.

Table 4. VFSMOD Inputs for pesticide mass balance and degradation calculations for the sample application

Inputs	Value	Units
<i>Water Quality (IWQ)</i>		
Partition coefficient (K_d)	0.396	L/Kg
% Clay in sediment (%CL)	25	%
IDG	1	(EU-FOCUS)
Pesticide degradation rate (k_{ref})	0.02475	day-1
Pesticide half-life ($t_{1/2} = \ln(2)/k_r$)	27.99	day
Soil field capacity (θ_{FC})	0.26	(-)
Incoming pesticide mass (m_i)	60970	mg
Mixing layer thickness (d_{mi})	2	cm
No. of days between events	3	
T(°C) (i=1,3)	9.5, 8.6, 6.3	
θ (-) (i=1,3)	0.265, 0.264, 0.265	

Other inputs

ISO: Porosity (OS)	0.42	(-)
IKW: Filter length (VL)	5	m
IKW: Filter width (FWIDTH)	100	m
IRO: Field length (SLENGTH)	100	m
IRO: Field width (SWIDTH)	100	m

Table 5. VFSSMOD outputs for pesticide mass balance and degradation calculations for the sample application

Inputs	Value	Units
<i>Water Quality (IWQ)</i>		
Phase distribution, Fph	994.266	
Infiltration (dQ)	48.17	%
Sediment reduction (dE)	99.918	%
Runoff inflow reduction	43.034	%
Pesticide reduction (dP)	63.804	%
<i>Water Balance (OSM)</i>		
Volume from rainfall (V_R)	17.35	m ³
Volume from up-field (V_i)	175.1	m ³
Volume from outflow (V_o)	99.75	m ³
Volume infiltrated (V_F)	92.7	m ³
<i>Sediment balance (OSM)</i>		
Sediment inflow (M_i)	444.7	Kg
Sediment outflow (M_o)	0.366	Kg
Sediment in filter	444.334	Kg

Specific calculations with the proposed equations are as follows:

$$m_o = m_i(1 - \Delta P) = 22068.70 \text{ mg}$$

$$\text{Eq. 4: } S_f = 0.1378 \text{ mg/Kg}$$

$$\text{Eq. 5: } m_f = 38901.30 \text{ mg}$$

$$\text{Eq: 6: } m_{f, sed} = 61.21 \text{ mg}$$

$$\text{Eq: 6: } m_{f, F} = 38840.09 \text{ mg}$$

$$\text{Eq 7: } C_F = 0.429 \text{ mg/L}$$

$$\text{Eq 10: } \rho_b = 1.5370 \text{ Kg/L}$$

$$\text{Eq 9: } m_m = 4.31 \text{ mg}$$

$$\text{Eq 11: } m_{res} |_{tend} = 65.52 \text{ mg}$$

$$\text{Eq 12-13: } m_{res} |_{tend} = 63.98 \text{ mg, with:}$$

day	$T(^{\circ}\text{C})$	$\theta(-)$	Eq. 13: $k(T,\theta)$	Eq. 12: m_{res} (mg)
0	--	--	--	65.52
1	9.5	0.265	0.009007	64.93
2	8.6	0.264	0.008262	64.40
3	6.3	0.265	0.006547	63.98

The final pesticide mass balance for the event and the residual amount at the beginning of the following event is depicted in Fig. 4.

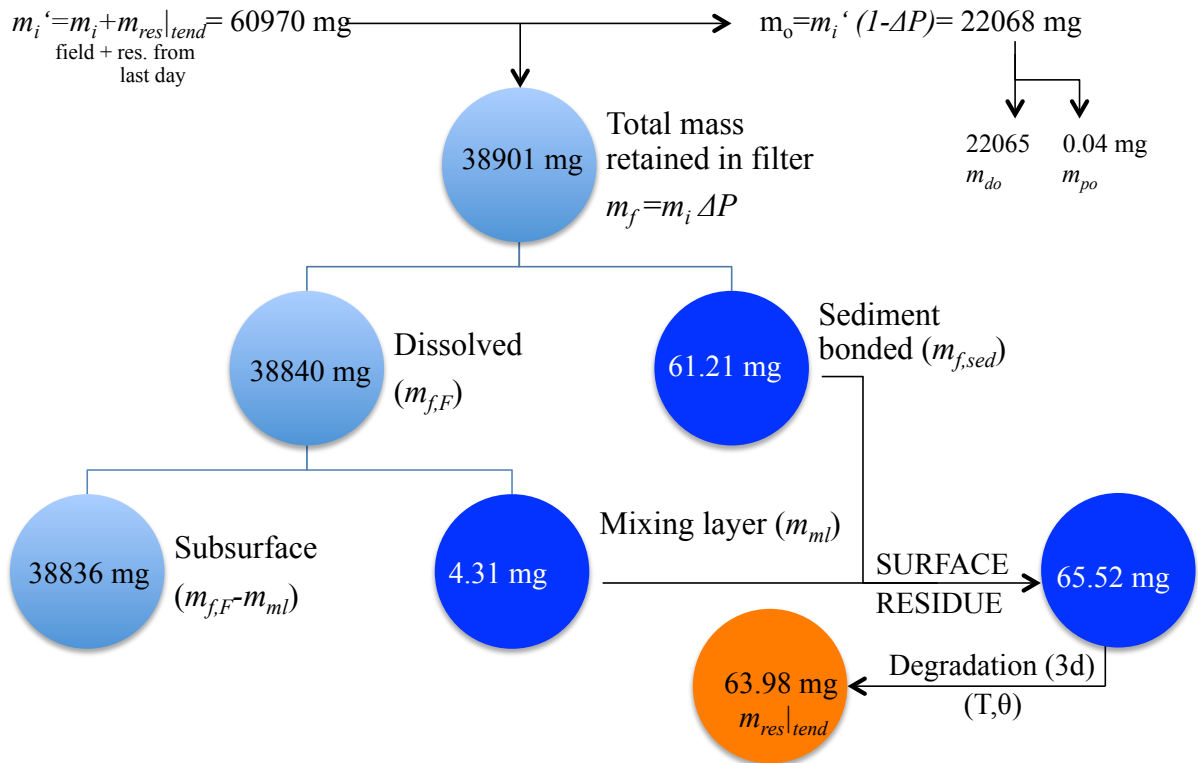


Figure 4. Partitioning of pesticide for sample application.

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LIST OF APPENDICES

APPENDIX A - Description of VFSSMOD degradation component

APPENDIX B- Soil and site parameters for EU FOCUS scenarios used in PRZM

APPENDIX A - Description of VFSSMOD pesticide degradation component

A.1 Structure of the IWQ file

```
IQPRO
IKD VKOC/VKD OCP
CCP
IDG
NDGDAY DGHALF FC DGPIN DGML
DGT(I)
DGTHETA(I)
```

A.2 Input factor definition

IWQPRO	Flag for type of water quality problem [=1 runs pesticides based on Sabbagh et al. (2009).; =2 runs simple solute transport (under construction); =3 runs the multireactive transport (under construction)]
IKD	Flag for reading VKOC, VKD and OCP. If IKD=0, then reads Kd; if IKD=1 then Koc and OCP are read.
VKOC	Adsorption coefficient (L/Kg)
VKD	Linear sorption coefficient (L/Kg)
OCP	% of organic carbon
CCP	% clay content in incoming sediment

[Factors used only if pesticide mass balance/residue calculation is requested (IDG=1-4)]

IDG	flag to calculate degradation (1-4, 1: EU: FOCUS, $k(k_{ref}, T, \theta)$; 2: US-EPA, $k=k_{ref}$; 3: $k=(k_{ref}, T)$; 4: $k=(k_{ref}, \theta)$), for other values ignore and no more lines needed.
NDGDAY	number of days between runoff events (from PRZM)
DGHALF	pesticide half-life (days) (at reference values of temperature and water content (i.e. 20°C and field capacity) (from PRZM). <u>Note:</u> $DGHALF=Ln(2)/DGKREF$
FC	θ_{FC} , topsoil field capacity (m^3/m^3). Values depend on the scenario definition. Appendix B provides values used in EU FOCUS R1-R4 scenario parameters used by PRZM field model.
DGPIN	total pesticide mass (liquid and solid phase) entering the filter per unit area of the source field (mg/m^2) (from PRZM + plus residual in filter calculated by VFSSMOD from last event in series, OWQ file). <u>Note:</u> this is converted to total mass entering at the filter as $m_i=DPIN*SLENGTH*SWIDTH$ (from IRO file)
DGML	d_{ml} , surface mixing layer thickness (cm). DGML=2 cm recommended (from PRZM)
DGT(I)	daily air temperatures (°C) for period between events, I=1, NDGDAY (from MET file)
DGTHETA(I)	top soil water content θ (m^3/m^3) for period between events, I=1, NDGDAY (from THETAFAO calculations based on MET file)

A.3 File Example

```

1          1 = read/create iwq & owq files
0 0.396    Kd proc.: 0= Kd(L/Kg); 1=Koc (Koc L/Kg) , %OC)
25        % Clay content in sediment
1         IDG
3 27.995 0.26 6.097E+00 2 ndgday dgHalf(d) FC(m3/m3) dgPin(mg/m2) dgML(cm)
9.5      8.6      6.3      (dgT(i),i=1,ndgday) (Celsius)
0.265    0.264    0.265    (dgTheta(i),i=1,ndgday (-)

```

A.2. OWQ Output file

The water quality output file in VFSMOD (OWQ) is modified when selecting the option IDG=1.

```

File: output/841215.owq                                VFSMOD v4.2.4 03/2014

Parameters for Water Quality
-----
                Type of problem= Pesticide trapping (Sabbagh et al.,2009)
Partition coefficient (Kd)=      0.396000          L/Kg
% Clay in sediment (%CL)=      25.000000          %
... Pesticide degradation requested
Pesticide half-life (Ln2/Kref)= 27.995000        days
Soil field capacity (FC)=      0.260000          (-)
Incoming pesticide mass (mi)=   6.097000        mg/m2
Mixing layer thickness (dml)=   2.000000        cm
No. of days between events=    3
                                day      T(C)   theta(-)
                                1      9.50000  0.26500
                                2      8.60000  0.26400
                                3      6.30000  0.26500

Outputs for Water Quality
-----
175.098 m3 = Runoff inflow
444.718 Kg = Sediment inflow
994.266     = Phase distribution, Fph
48.170 %   = Infiltration (dQ)
99.919 %   = Sediment reduction (dE)
43.034 %   = Runoff inflow reduction

63.804 %   = Pesticide reduction (dP)

Pesticide mass balance/degradation (IDG=1)
-----
Total mass in filter:

0.609700E+05 mg = Pesticide input (mi)
0.220686E+05 mg = Pesticide output (mo)
0.612102E+02 mg = Pesticide retained in filter, sediment-bonded, (mf,sed)
0.430983E+01 mg = Pesticide retained in filter, mixing layer (mml)
0.655201E+02 mg = Pesticide surface residue at the end of this event (mres)
0.639781E+02 mg = Pesticide surface residue at next event (after degradation, 3 days)

Normalized values by source area:

10000.00 m^2 = Source Area (input)
0.609700E+01 mg/m2= Pesticide input (mi)
0.220686E+01 mg/m2= Pesticide output (mo)
0.612102E-02 mg/m2= Pesticide retained in filter, sediment-bonded (mf,sed)
0.430983E-03 mg/m2= Pesticide retained in filter, mixing layer (mml)
0.655201E-02 mg/m2= Pesticide surface residue at the end of the event (mres)
0.639781E-02 mg/m2= Pesticide surface residue at next event (after degradation, 3 days)

Pesticide mass partition for outflow

0.316647E-01 mg = Pesticide output in solid phase (mop)
0.220685E+05 mg = Pesticide output in liquid phase (mod)

```

APPENDIX B - Soil and site parameters for EU FOCUS scenarios used in PRZM

The field capacity (FC) for the top soil (Ap) is the value required as an input in the IWQ file.
Note: the units required in IWQ are not percentage, but fractional units (i.e. 33.8% would be 0.338 in IWQ).

Table 6. R1 soil and site parameters for PRZM (Table D-14 in EU FOCUS manual)

Horizon (FAO, 1990) Depth (cm)	Ap 0-30	Bw 30-60	BC 60-100+
BASIC PROPERTIES			
Sand (%)	5	6	5
Silt (%)	82	83	84
Clay (%)	13	11	11
Texture (FAO, 1990; USDA, 1999)	silt loam	silt loam	silt loam
Organic carbon (%)	1.2	0.3	0.1
Bulk density (g/cm ³)	1.35	1.45	1.48 ^a
PH	7.3	7.6	8.0
Structure (FAO, 1990) Development Size Shape	Weak Fine Subangular blocky	Weak Medium Subangular blocky	Very weak Very coarse Subangular blocky
HYDRAULIC PROPERTIES			
Field capacity (% volume)	33.8 ^b	28.6 ^b	27.7 ^b
Wilting point (% volume)	14.1 ^b	11.1 ^b	10.8 ^b
RUNOFF & SOIL LOSS PROPERTIES			
Parameter	Value	Selection criteria	Reference
Hydrologic group (HGRP)	C	appropriate for soil type	FOCUS definition
USLE K factor (USLEK)	0.42	silt/silt loam, 2% OM	PRZM manual
USLE LS factor (USLELS)	0.33	45 m length, 3% slope	PRZM manual
USLE P factor (USLEP)	0.50	contouring, 3% slope	PRZM manual
Area of field (AFIELD)	0.45 ha	assumption for scenario	FOCUS definition
IREG	3	even monthly rain distrib.	FOCUS definition
Slope (SLP)	3%	appropriate for scenario	FOCUS definition
HL	20 m	assumption for scenario	FOCUS definition
Manning's coefficient	0.10	fallow, no-till or coultur	PRZM manual

^a Estimated value using SSLRC algorithms and measured local data for the soil type.

^b Calculated using PRZM pedo-transfer functions with other data given in the table
 (FC = -33 kPa; WP = -1500 kPa).

Table 7. R2 soil and site parameters for PRZM (Table D-15 in EU FOCUS manual)

Horizon (FAO, 1990) Depth (cm)	Ap 0-20	Ah 20-45	AB1 45-65	AB2 65-100
BASIC PROPERTIES				
Sand (%)	67	72	75	74
Silt (%)	19	16	13	16
Clay (%)	14	12	12	10
Texture (FAO, 1990; USDA, 1999)	sandy loam	sandy loam	sandy loam	sandy loam
Organic carbon (%)	4.0	2.4	0.8	0.5 ^a
Bulk density (g/cm ³)	1.15 ^b	1.29 ^b	1.36 ^b	1.41 ^b
pH	4.5	4.9	5.4	5.3
Structure (FAO, 1990) Development Size Shape	Moderate Medium Subangular blocky	Weak Medium Subangular blocky	Weak Medium Subangular blocky	Weak Medium Subangular blocky
HYDRAULIC PROPERTIES				
Field capacity (% volume)	36 ^c	27 ^c	19 ^c	17 ^c
Wilting point (% volume)	18 ^c	14 ^c	10 ^c	8 ^c
RUNOFF & SOIL LOSS PROPERTIES				
Parameter	Value	Selection criteria	Reference	
Hydrologic group (HGRP)	B / C	appropriate for soil type	FOCUS definition	
USLE K factor (USLEK)	0.19	sandy loam, 4% OM	PRZM manual	
USLE LS factor (USLELS)	0.66	45 m length, 5% slope	PRZM manual	
USLE P factor (USLEP)	0.50	contouring, 5% slope	PRZM manual	
Area of field (AFIELD)	0.45 ha	assumption for scenario	FOCUS definition	
IREG	2	heavier winter rain	FOCUS definition	
Slope (SLP)	5%	20% slope, terraced to 5%	FOCUS definition	
HL	20 m	assumption for scenario	FOCUS definition	
Manning's coefficient	0.10	fallow, no-till or coulters	PRZM manual	

^a Estimated value based on horizon type and value for horizon above.

^b Estimated value using SSLRC algorithms and measured local data for the soil type.

^c Calculated using PRZM pedo-transfer functions with other data given in the table
(FC = -33 kPa; WP = -1500 kPa).

Table 8. R3 soil and site parameters for PRZM (Table D-16 in EU FOCUS manual)

Horizon (FAO, 1990) Depth (cm)	Ap1 0 – 45	Ap2 45 - 75	Bk 75 – 145	C 145 – 160
BASIC PROPERTIES				
Sand (%)	23	25	17	14
Silt (%)	43	42	48	50
Clay (%)	34	33	35	36
Texture (FAO, 1990; USDA, 1999)	clay loam	clay loam	silty clay loam	silty clay loam
Organic carbon (%)	1.0	1.0	0.35	0.29
Bulk density (g/cm ³)	1.46 ^a	1.49 ^a	1.52 ^a	1.54 ^a
pH	7.9	7.9	8.3	8.6
Structure (FAO, 1990) Development Size Shape	Moderate fine Granular	Moderate Fine granular	Weak coarse Subangular blocky	Weak Very coarse Angular blocky
HYDRAULIC PROPERTIES				
Field capacity (% volume)	37 ^b	35 ^b	36 ^b	36 ^b
Wilting point (% volume)	22 ^b	21 ^b	21 ^b	22 ^b
RUNOFF & SOIL LOSS PROPERTIES				
Parameter	Value	Selection criteria		Reference
Hydrological group (HGRP)	C	appropriate for soil type		FOCUS definition
USLE K factor (USLEK)	0.25	clay loam, 1% OM		PRZM manual
USLE LS factor (USLELS)	0.66	45 m length, 5% slope		PRZM manual
USLE P factor (USLEP)	0.50	contouring, 5% slope		PRZM manual
Area of field (AFIELD)	0.45 ha	assumption for scenario		FOCUS definition
IREG	3	even seasonal rain		FOCUS definition
Slope (SLP)	5%	10% slope, terraced to 5%		FOCUS definition
HL	20 m	assumption for scenario		FOCUS definition
Manning's coefficient	0.10	fallow, no-till or coultur		PRZM manual

^a Estimated using SSLRC pedo-transfer functions with other data given in the table and checked against data in the PRZM manual.

^b Calculated using PRZM pedo-transfer functions with other data given in the table (FC = -33 kPa, WP = -1500 kPa).

Table 9. R4 soil and site parameters for PRZM (Table D-17 in EU FOCUS manual)

Horizon (FAO, 1990) Depth (cm)	Ap1 0-30	Ap2 30-60	2C1 60 - 170	2C2 170-300
BASIC PROPERTIES				
Sand (%)	53	53	69	65
Silt (%)	22	22	24	27
Clay (%)	25	25	7	8
Texture (FAO, 1990; USDA, 1999)	sandy clay loam	sandy clay loam	sandy loam	sandy loam
Organic carbon (%)	0.6	0.6 ^a	0.08	0.08
Bulk density (g/cm ³)	1.52	1.50 ^a	1.49	1.50
pH	8.4	8.4 ^a	8.8	8.8
Structure (FAO, 1990) Development Size Shape	Moderate Fine Subangular blocky	Moderate Fine Subangular blocky	Apedal N/A Single grain	Apedal N/A Single grain
HYDRAULIC PROPERTIES				
Field capacity (% volume)	26 ^b	27 ^b	14.5 ^b	16 ^b
Wilting point (%volume)	16 ^b	16 ^b	6 ^b	7 ^b
RUNOFF & SOIL LOSS PROPERTIES				
Parameter	Value	Selection criteria		Reference
Hydrologic group (HGRP)	C	appropriate for soil type		FOCUS definition
USLE K factor(USLEK)	0.26	sandy clay loam, 0.6% OM		PRZM manual
USLE LS factor (USLELS)	0.66	45 m length, 5% slope		PRZM manual
USLE P factor (USLEP)	0.50	contouring, 5% slope		PRZM manual
Area of field (AFIELD)	0.45 ha	assumption for scenario		FOCUS definition
IREG	2	heavier winter rain		FOCUS definition
Slope (SLP)	5%	appropriate for scenario		FOCUS definition
HL	20 m	assumption for scenario		FOCUS definition
Manning's coefficient	0.10	fallow, no-till or coulters		PRZM manual

^a Estimated value based on horizon type and value for horizon above.

^b Calculated using PRZM pedo-transfer functions with other data given in the table (FC = -33 kPa; WP = -1500 kPa).