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

R. Muñoz-Carpena, Ph.D.

Agricultural and Biological Engineering

University of Florida

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Photo: http://www.irisa.fr/bunraku/GENS/kboulang/images/parkground.png
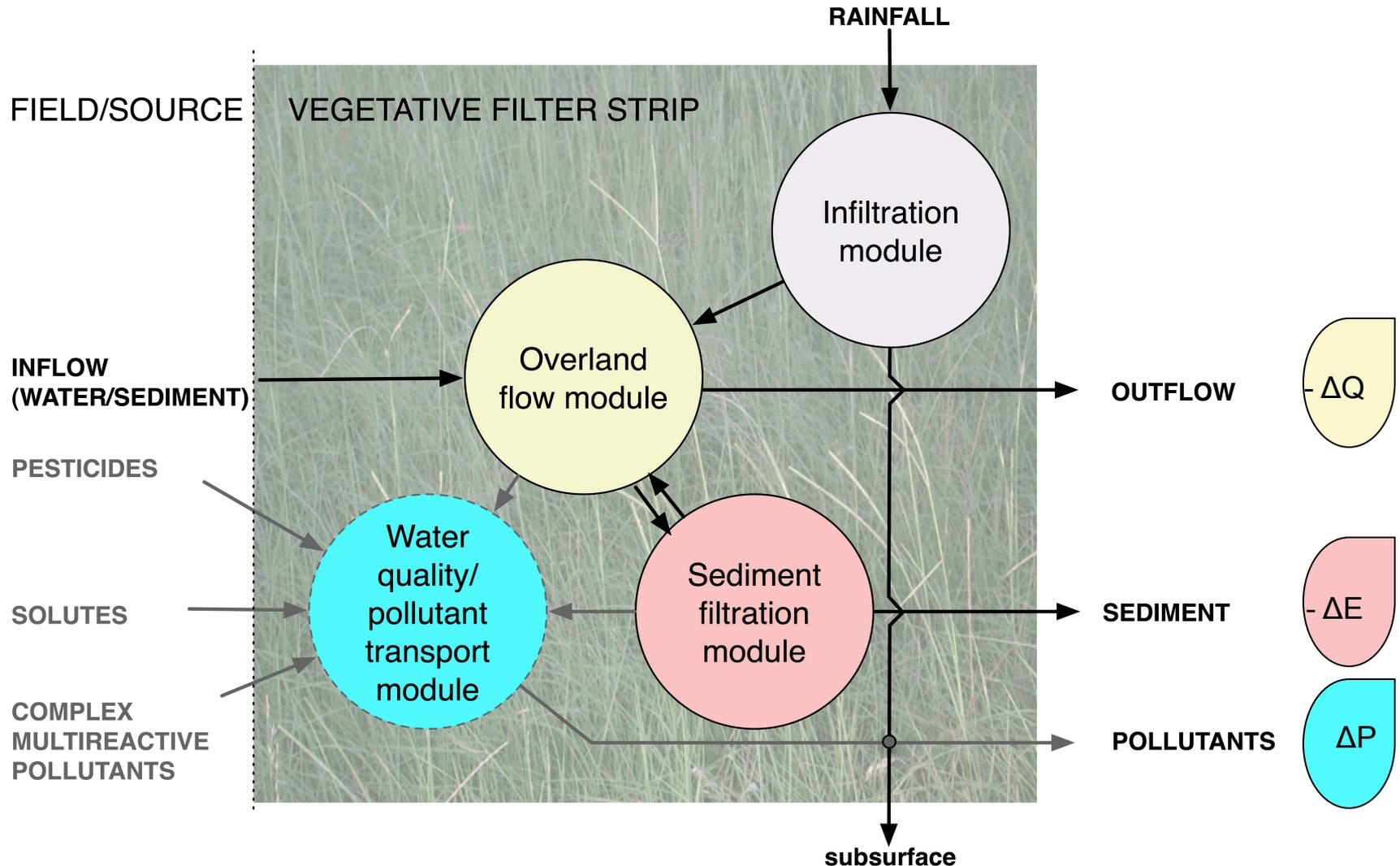
Scope/Objectives

- Evaluation of the VFS effects on the long-term pesticide assessment simulations require realistic initial conditions at the beginning of each runoff event in the time series (initial soil water, pesticide residue and vegetation status).

- A new procedure based on FAO-56 is developed to calculate the filter strip topsoil water content dynamics between runoff events. This yields VFSMOD's OI parameter at the beginning of each runoff event in the long-term environmental assessment time series

- A simplified VFS pesticide mass balance is proposed to estimate surface pesticide residue for inclusion in VFSMOD's buffer efficiency calculations.
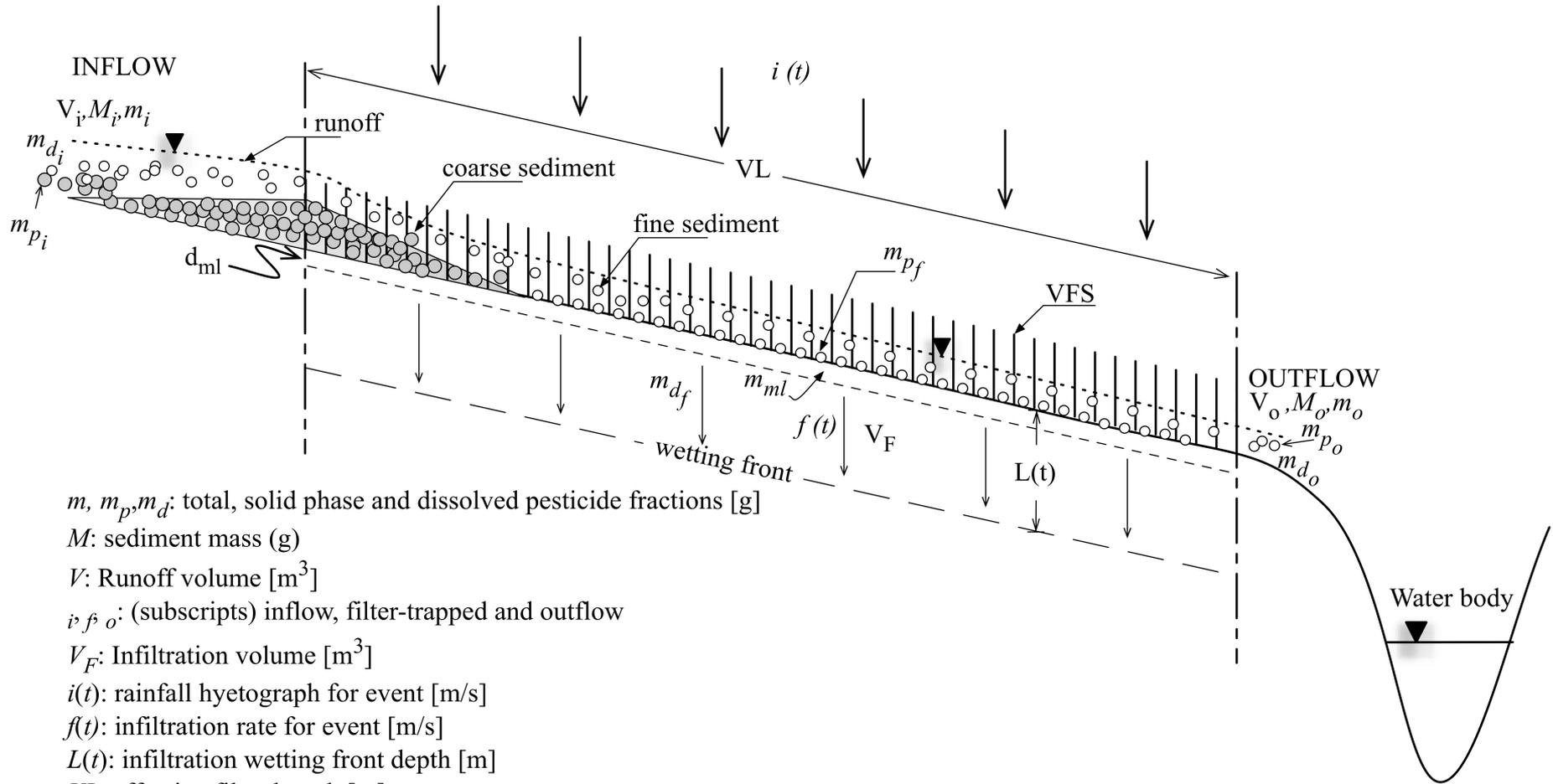
1. Surface pesticide mass balance and residue

Scope/Rationale

1. Focus of simplified mass balance is on surface pesticide trapping and transport through the filter

   – Dissolved pesticide trapped through infiltration and moved to the subsurface is calculated but not considered for degradation towards next runoff event in time

2. Residual pesticide attached to sediment trapped on the filter after the event is handled as a worst-case scenario where all mass is available for degradation and transport (and trapping) towards the next event.
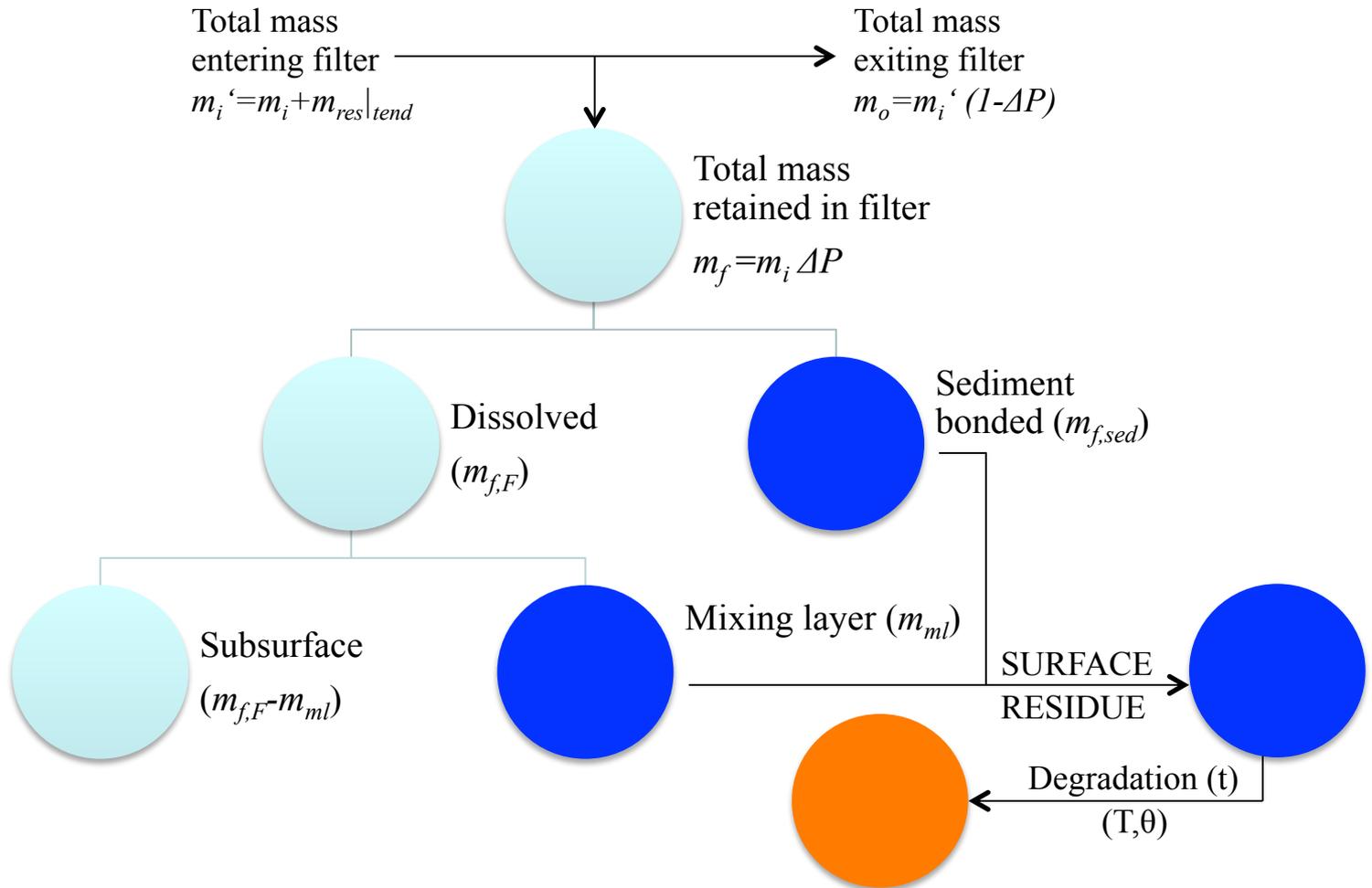
VFSMOD: dynamic flow and sediment

FIELD/SOURCE — VEGETATIVE FILTER STRIP

RAINFALL

Infiltration module

Overland flow module

INFLOW (WATER/SEDIMENT)

OUTFLOW — ΔQ

PESTICIDES

Water quality/ pollutant transport module

Sediment filtration module

SEDIMENT — ΔE

SOLUTES

COMPLEX MULTIREACTIVE POLLUTANTS

POLLUTANTS — ΔP

subsurface

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http://abe.ufl.edu/carpena/vfsmod

[*Muñoz-Carpena, et al.*, 1993b; 1999, 2004]

Conceptual mass balance

INFLOW

V_i, M_i, m_i

m_{d_i}

m_{p_i}

runoff

d_{ml}

coarse sediment

fine sediment

$i\,(t)$

VL

m_{p_f}

VFS

m_{d_f} m_{ml}

$f\,(t)$ V_F

wetting front

L(t)

OUTFLOW
V_o, M_o, m_o

m_{p_o}

m_{d_o}

Water body

m, m_p, m_d: total, solid phase and dissolved pesticide fractions [g]

M: sediment mass (g)

V: Runoff volume [m^3]

$_i, _f, _o$: (subscripts) inflow, filter-trapped and outflow

V_F: Infiltration volume [m^3]

$i(t)$: rainfall hyetograph for event [m/s]

$f(t)$: infiltration rate for event [m/s]

$L(t)$: infiltration wetting front depth [m]

VL: effective filter length [m]

d_{ml}: surface mixing layer depth [m]

Coarse sediment: particle diameter >0.037 mm (bed load transport)

Fine sediment: particle diameter <0.037 mm (suspended load transport)

Conceptual mass balance - Residue

Total mass entering filter
$m_i{'}=m_i+m_{res}|_{tend}$

Total mass exiting filter
$m_o=m_i{'}\ (1-\Delta P)$

Total mass retained in filter
$m_f=m_i\ \Delta P$

Dissolved $(m_{f,F})$

Sediment bonded $(m_{f,sed})$

Subsurface $(m_{f,F}-m_{ml})$

Mixing layer (m_{ml})

SURFACE RESIDUE

Degradation (t) (T,θ)

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Pesticide partitioning (1)

1. For each event in time series field model (PRZM, other) provides total mass of incoming pesticide into the filter

   – Central assumption: solid phase concentration (incoming, in filter, and outgoing) at equilibrium, i.e. does not change during event ➔ $S_i \approx S_f \approx S_o$

   – Equilibrium between runoff dissolved and solid phase is assumed and pesticide is partitioned using K_d value for the pesticide,

   $$K_d = \frac{S_i}{C_i} = \frac{m_{p_i}/M_i}{m_{d_i}/V_i} \Rightarrow S_i = \frac{m_i K_d}{V_i + M_i K_d} \approx S_f \approx S_o$$

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Pesticide partitioning (2)

2. Similarly, for each event dissolved and particulated pesticide left in the filter and transported through is calculated using equilibrium assumptions (K_d) based on VFSMOD I/O for water and sediment mass balance

3. The sediment-adsorbed fraction deposited on the VFS surface during the event can be estimated proportional to the sediment mass deposited in the filter,

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

Pesticide partitioning (3)

4. 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,

$$m_{ml} = m_{ml_d} + m_{ml_p} \approx \left(\theta_s C_F + \rho_b S \right) V_{ml} = \left(\theta_s + K_d \rho_b \right) C_F d_{ml}.b.VL$$

4. The mixing layer dissolved pesticide from the infiltration component is considered part of the surface residual mass for pesticide degradation calculations.

Pesticide degradation (1)

1. To calculate the residual mass at the beginning of the next runoff event, 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) taking into account daily average temperature and soil moisture (FOCUS group, 1996; EFSA opinion 11/03/2009),

$$\frac{dm_{res}}{dt} = -k.m_{res} \Rightarrow m_{res}\big|_{t_1} = m_{res}\big|_{t_0} e^{-kt}$$

$$k(T,\theta) = k_{ref} e^{\frac{E_a}{R}\left(\frac{1}{T_{ref}} - \frac{1}{T}\right)} \left(\frac{\theta}{\theta_{ref}}\right)^{-\beta}$$

m_{res}: residual mass in the filter (M)
t= time (days)
T= average surface soil (≈air) temperature (K) between events
θ= average surface soil moisture between events
k=k(T, θ)=pesticide half-life adjusted for (T, θ) (days)
k_{ref}= pesticide half-life (days) (at reference values of T and θ)
E_a= degradation activation energy, 65.4 kJ/mol (10-90 kJ/mol)
R= gas constant, 8.314 J/mol/K
β= constant (rec. 0.7, FOCUS v2.0, 2006)

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Pesticide degradation (2)

3. Soil temperature is only considered on the top soil mixing layer (d_{ml}=0.5-5 cm). Based on heat transport equation, the air temperature attenuates and delays in time through the soil profile until reaching a constant temperature deep in the profile. Thus, a reasonable approximation for a thin surface layer, $T_{top} \approx T_{air}$

4. Top soil moisture (θ) is estimated based on FAO-56 crop coefficient method (FAO, 1998) when ET and atmospheric parameters are known (from FOCUS SW scenario) (Report 1).

Pesticide degradation (3)

3. 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 (m'_i). 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 obtained the outflow total pesticide mass leaving the filter in runoff at the end of the event,

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

Assumptions of pesticide mass balance/degradation component

Component	Assumptions/Limitations
Pesticide mass balance	☒ 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	☒ 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)	☒ All residual mass in mixing layer after degradation is added to new field incoming mass for next event in time series

VFSMOD new input requirements

All inputs are provided in the revised EU SWAN (PRZM/ VFSMOD) framework

Input	Source	Comment
nday	PRZM	No. days to next runoff event
T_j (j=1,nday)	FOCUS	Degradation equation
θ_j (j=1,nday)	THETAFAO/Shell	From MET file info: ETP, PRECIP,WIND,Tmax,Tmin
k_{ref}	PRZM	Degradation equation
FC	PRZM	Degradation equation
d_{ml}	Recomm. PRZM (2 cm)	Pesticide mass balance
m'_i	PRZM+ VFSMOD (previous event)	Runoff pesticide mass entering filter

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Revised IWQ input file

```
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 (-)
```
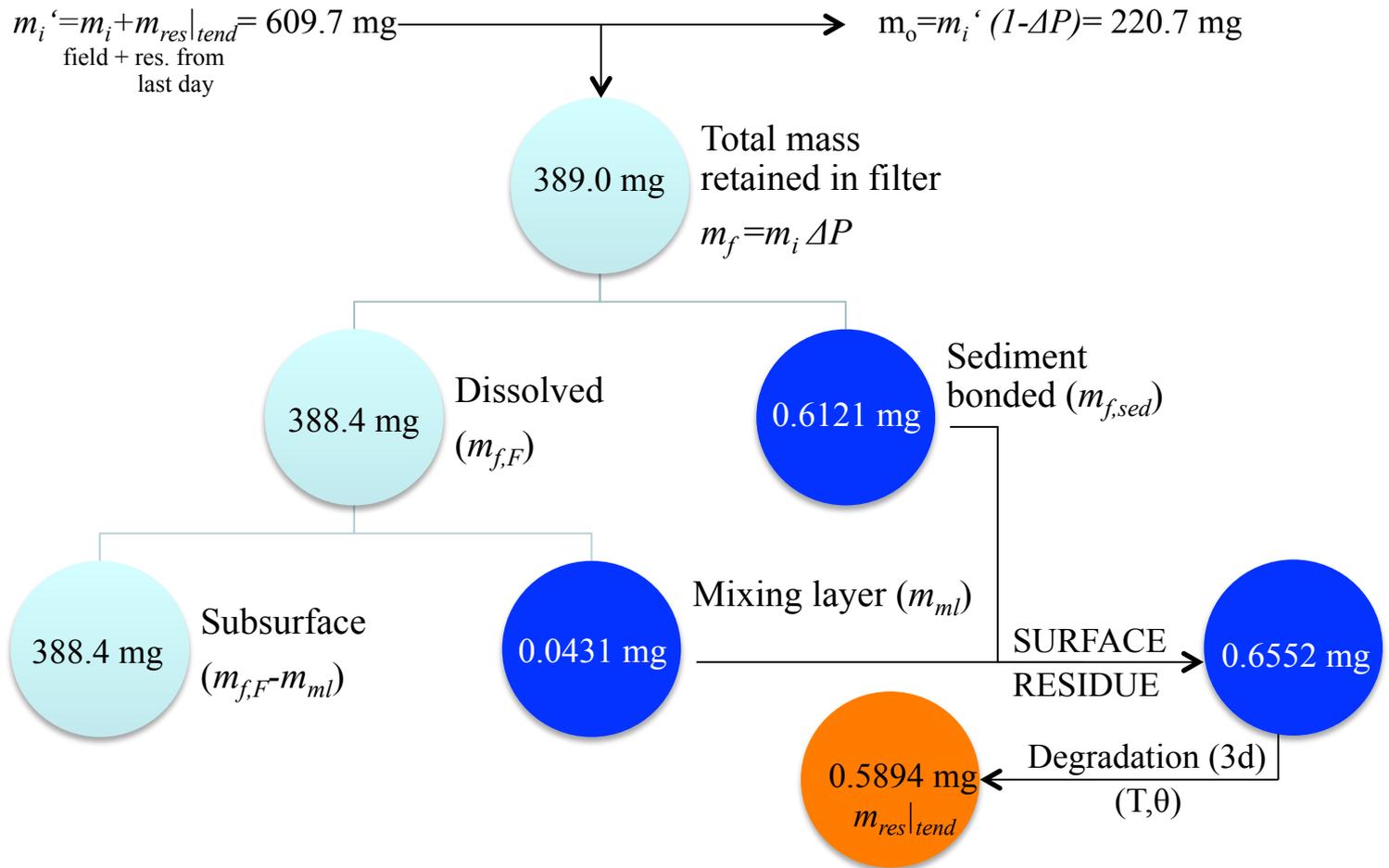
## Where the new factors in lines 3-6 are:

IDG   flag to calculate degradation (1, other ignore).

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).

FC $\theta_{FC,}$ 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 ($mg/m2$) (from PRZM + plus residual in filter calculated by VFSMOD from last event in series, OWQ file). Note: 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 (m^3/m^3) for period between events, I=1,NDGDAY (from THETAFAO calculations based on MET file)

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Conceptual mass balance - Example

$m_i{}'=m_i+m_{res}|_{tend}= 609.7$ mg $\longrightarrow$ $m_o=m_i{}'\,(1-\Delta P)= 220.7$ mg

field + res. from last day

389.0 mg

Total mass retained in filter

$m_f=m_i\,\Delta P$

388.4 mg — Dissolved ($m_{f,F}$)

0.6121 mg — Sediment bonded ($m_{f,sed}$)

388.4 mg — Subsurface ($m_{f,F}-m_{ml}$)

0.0431 mg — Mixing layer (m_{ml})

SURFACE RESIDUE

0.6552 mg

0.5894 mg $m_{res}|_{tend}$ ← Degradation (3d) (T,θ)

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Filter length change & maintenance

1. The sediment deposition at the end of the event can degrade the filter over time and quickly after major runoff events (see sediment wedge in slides 6, 19).

2. VFSMOD can be set to rewrite the geometry file of the filter (*.ikw) after each event to account for this (change in Manning's n in front of filter, effective length from then end of the top of the trapezoidal wedge).

3. If this option is selected, a maintenance cycle must be set by the user (i.e. a reset to the original grass and geometry at t=0 every so many years).
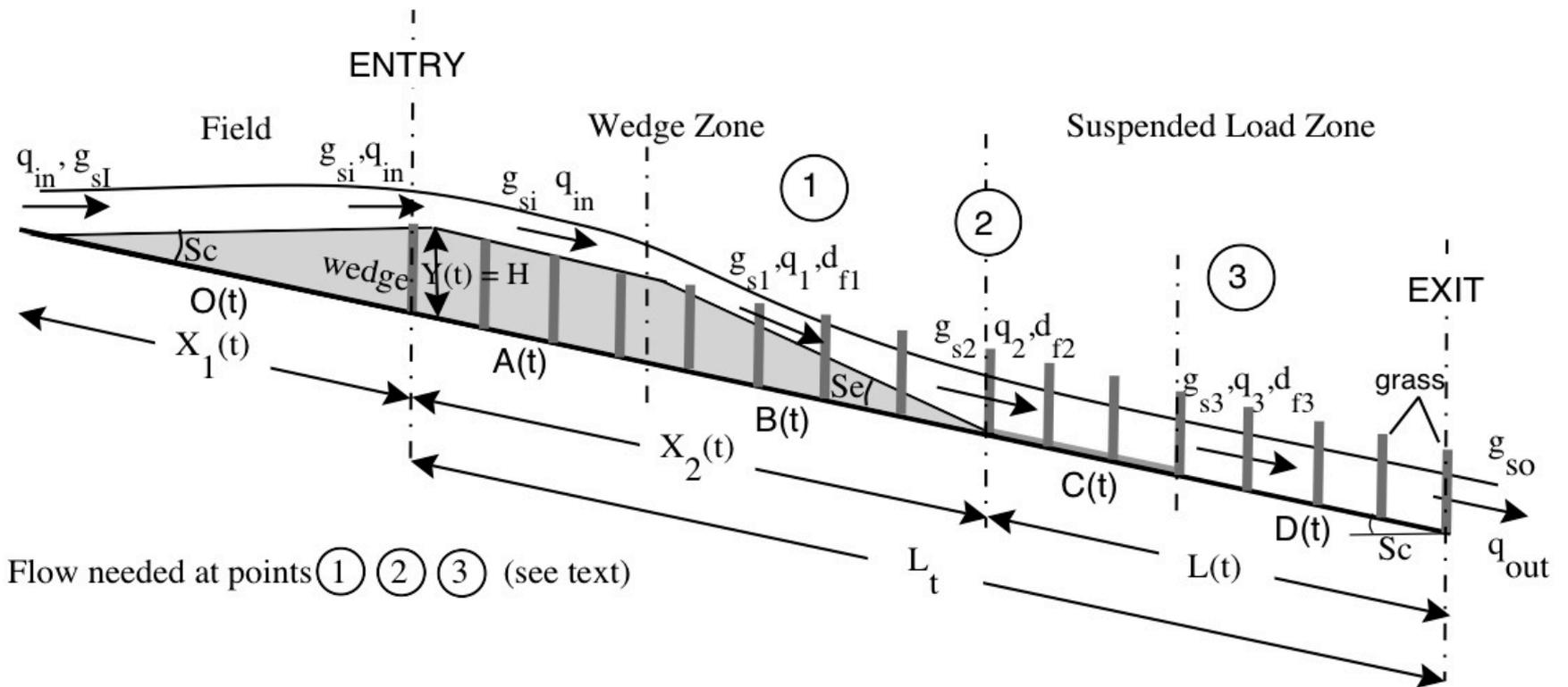
2. Soil water dynamics in VFS for long-term assessments

# Estimation of VFS top soil moisture for continuous simulation

- FAO-56 single crop coefficient method (FAO, 1998), relatively simple computationally, is intended to improve daily simulation of actual crop evapotranspiration (ET_a) by considering separately the contribution of vegetation and water stress (soil) factors,
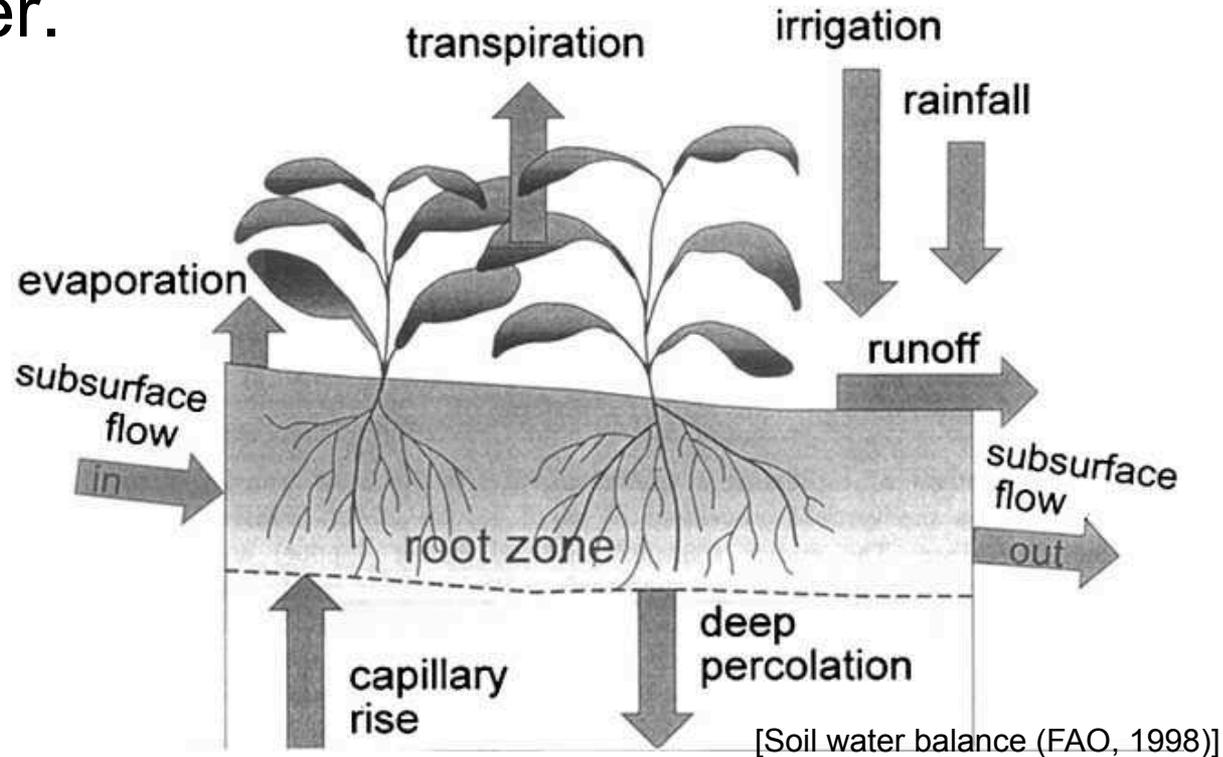
$$ET_a = K_c\, K_s\, ET_o$$

(crop factor) $$K_c = K_{c,mid} + [0.04(u_2 - 2) - 0.004(RH_{min} - 45)]\left(\frac{h}{3}\right)^{0.3}$$

θ : soil water content

(stress factor) $$K_s = \begin{cases} \dfrac{TAW - D_{r,i}}{TAW - RAW} = \dfrac{TAW - D_{r,i}}{(1-p)TAW} & D_{r,i} > RAW \\[2mm] 1 & D_{r,i} \leq RAW \end{cases}$$

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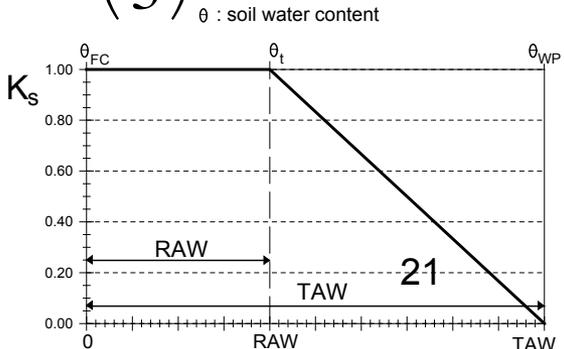
- Used inversely through the soil water (mass) balance principle it is possible to predicts the daily soil water content (θ_i) in the soil surface layer.
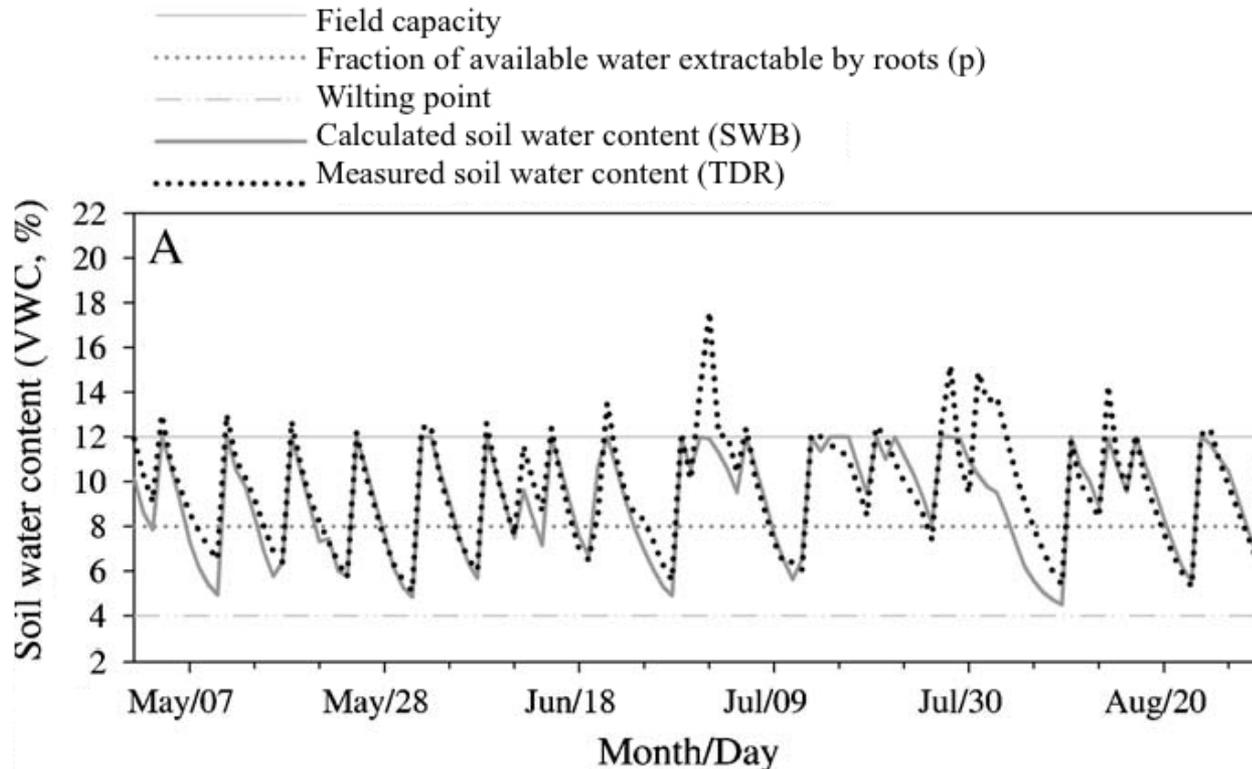

[Soil water balance (FAO, 1998)]

$$\Delta\theta_i = \theta_i - \theta_{i-1} = P_i - ET_i - DP_i \; ; \; D_{r,i} = D_{r,i-1} - P_i + ET_{c,i} + DP_i$$

- Method estimates root zone soil water (θ) dynamics based on readily available weather (ET_o, rain, wind and temperature) and soil and vegetation characteristics (provided by the FOCUS/PRZM framework or tabulated in the original FAO-56).

- On going testing with pesticide field degradation experiments at IRSTEA (formerly CEMAGREF) in Lyon

- A simplified calculation procedure, and implementation in VFSMOD are detailed in the report developed for this project available at,

http://abe.ufl.edu/carpena/vfsmod/FOCUSreports.shtml

- Good comparison with field measured topsoil water content measured with dielectric probes in McCready and Dukes (2011) and in previous work at UPM Madrid, Prof. Miguel Quemada.

Example of soil volumetric content calculated daily using the soil water balance on well-established warm season grass with 30 cm root depth (adapted from Fig. 2 on McCready and Dukes, 2011).

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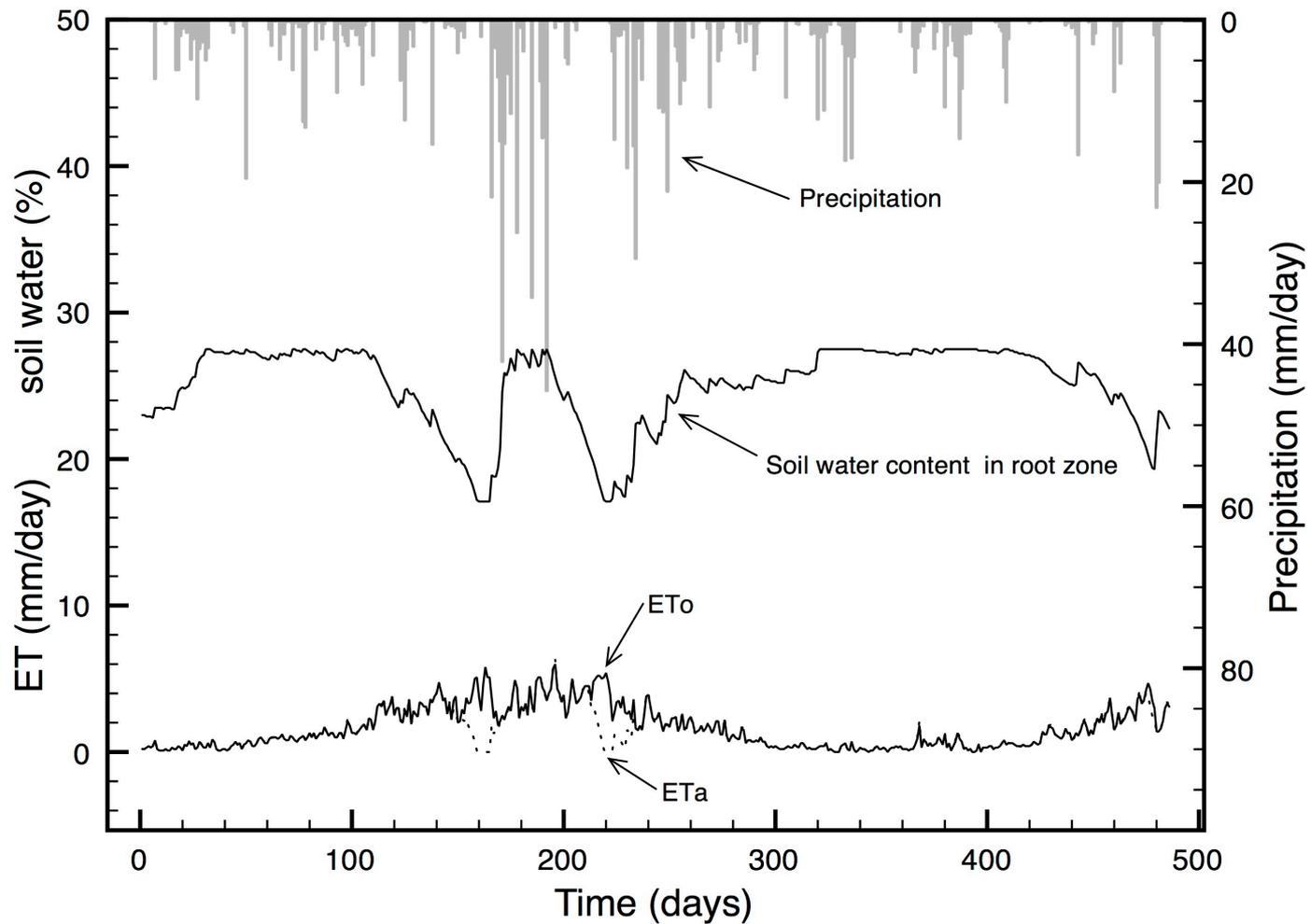
Example calculation of VFS root zone soil water variation between storms for the example case (Bermuda grass, EU FOCUS R1 scenario conditions, loamy soil).