Impact of step 4 scenario assumptions and VFSMOD parameterisation on the effectiveness of vegetative filter strips in reducing PEC in surface water

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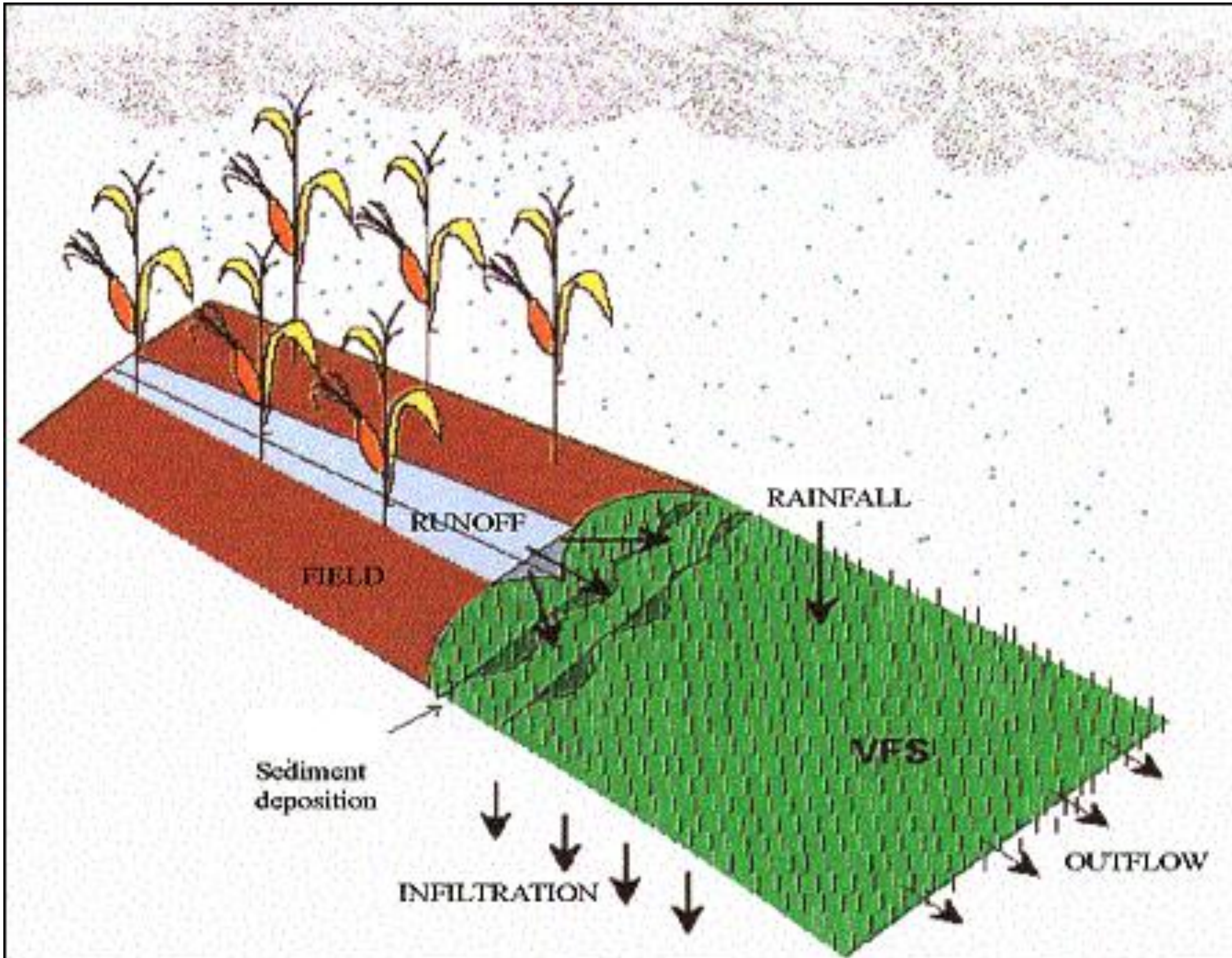
1. Introduction



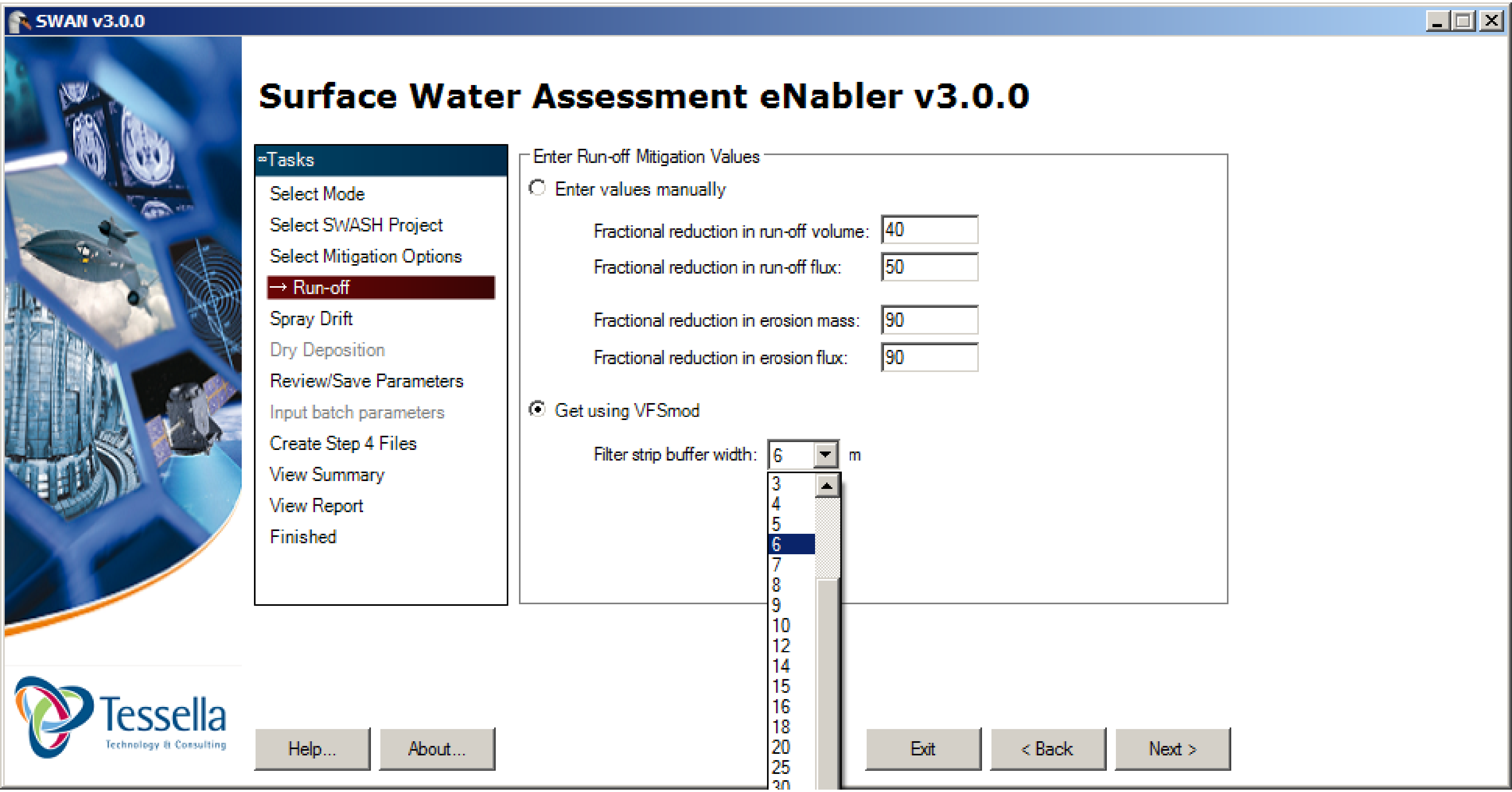
Introduction: VFSMOD (1)

- VFSMOD (e.g. Muñoz-Carpena und Parsons, 2011; http://abe.ufl.edu/carpena/vfsmod/) is a numerical model for the dynamic simulation of vegetated filter strips (VFS)
- Various versions
  - vfsm.exe: command line
  - VFSMOD-W: Windows shell + vfsm.exe
  - SWAN-VFSMOD (developed by ECPA for FOCUS step4) with VFSMOD as .dll
- Main characteristics of VFSMOD
  - 1 simulation = 1 surface runoff event
  - mechanistic simulation of infiltration and sedimentation
  - reduction of pesticide load with a multiple regression equation (Sabbagh et al., 2009); deltaP = f(deltaE, deltaQ, Fph, C)
  - mechanistic solute transport implemented in a research version (Perez-Ovilla, 2010)
- Relevant outputs:
  - deltaQ: relative reduction of total incoming water flow (incoming surface runoff + rainfall on VFS)
  - deltaR: relative reduction of incoming surface runoff
  - deltaE: relative reduction of incoming sediment load
  - deltaP: relative reduction of incoming pesticide load

Introduction: VFSMOD (2)

- Newer versions of VFSMOD are able to simulate shallow water tables (Muñoz-Carpena et al., 2011).
- This feature is especially relevant for VFS adjacent to surface water bodies or for soils with poorly permeable or impermeable horizons.
- 4 lower boundary conditions
  - no water table simulated (BC0)
  - water table with Dupuit-Forchheimer assumptions (BC1) (recommended by Rafael Muñoz-Carpena as "most relevant in field situations")
  - water table with vertical saturated flow (BC2)
  - water table with simplified method (BC3)

Introduction: SWAN-VFSMOD



Introduction: SWAN-VFSMOD

- SWAN 3.0 contains two options:
  a) user-defined fixed efficiencies of VFS (inherited from SWAN v. 1)
  b) dynamic simulation of VFS (SWAN-VFSMOD)
- many events in one p2t file → many VFSMOD runs per p2t file
  - long time simulations of soil moisture in advance using the tool ThetaFAO (Muñoz-Carpena, 2012a)
  - carry-over of residues from one surface runoff event to the next (Muñoz-Carpena, 2012b)
  - however: no ageing (e.g. progressive silting up) of the buffer strip is simulated: the VFS is assumed to be maintained between events so that it is in perfect condition at the start of each event
- Advantage of SWAN-VFSMOD: more realistic simulation of VFS efficiency than with fixed efficiency values
- Disadvantage: SWAN-VFSMOD cannot fix the main problems inherent in FOCUSsw, especially the lack of representativeness of the simulated 12-month period
- Further critical assumption in SWAN (1.x and 3.0): The non-treated (with the simulated pesticide!) area of the upstream catchment of the FOCUS stream (80 % of 100 ha) doesn't have buffer strips → relatively high dilution with the unchanged surface runoff volumes from these areas

2. Effect of scenario assumptions outside VFSMOD

Equation of Ter Horst et al. (2009) for FOCUS stream

$$PECsw\max, step4 = \frac{21(1 - frvf)M}{80V + 21(1 - frvf)V}$$

with

M	pesticide runoff flux leaving the field (PRZM output)
V	surface runoff volume leaving the field (PRZM output)
frvf	fractional reduction of both surface runoff volume (frv = deltaR/100) and pesticide runoff flux (frf = deltaP/100) due to the buffer strip

- Underlying assumptions: baseflow, standing water volume and lateral subsurface flow negligible compared with surface runoff volume entering the stream
- Conclusion: In SWAN the relative reduction in PECsw,max compared with the standard FOCUS step3 simulation is approximately equal to frvf.

Deriving analytical relationship for deltaPECsw

- In the following, we try to generalize the special case of Ter Horst et al. (2009):
  1) we remove the assumption that frv = frf, because with VFSMOD this is usually not the case,
  2) we remove the SWAN assumption that the treated fraction of the upstream catchment (ft) is equal to the fraction equipped with buffer strips (fb).
- Derive PECswmax,step4 (PRZM-VFSMOD-TOXSWA) and relate it to PECswmax,step3 (PRZM-TOXSWA) in order to calculate the relative reduction deltaPECsw.
- The derivation is described in Reichenberger and Pires (2014; report available in pdf format)

Analytical relationship for deltaPECsw (FOCUS stream)

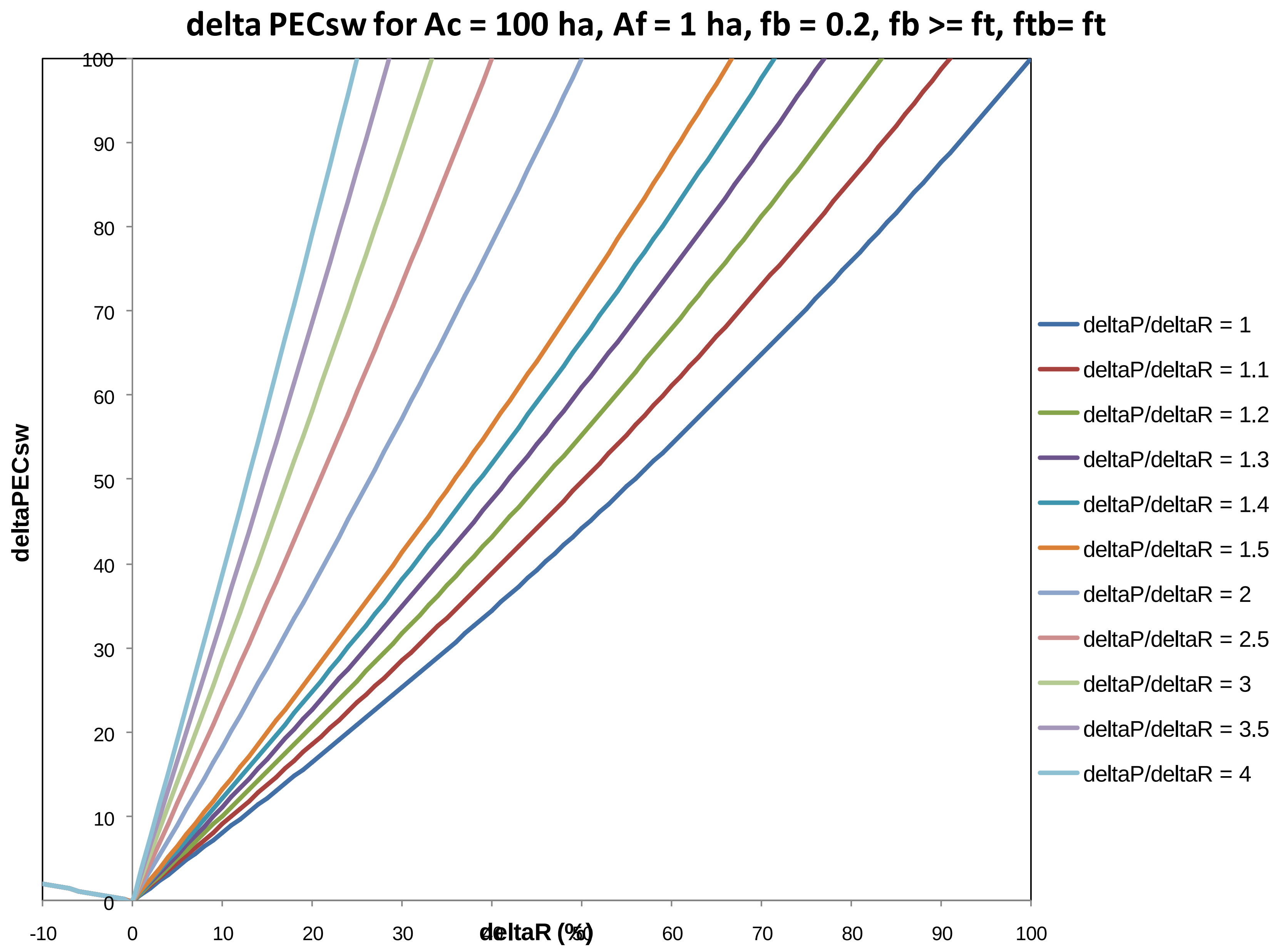
$$deltaPECsw = (1 - \frac{(1 - frf)*(Ac + Af)}{(Ac * fb + Af)(1 - frv) + (1 - fb)Ac})*100\%$$

with

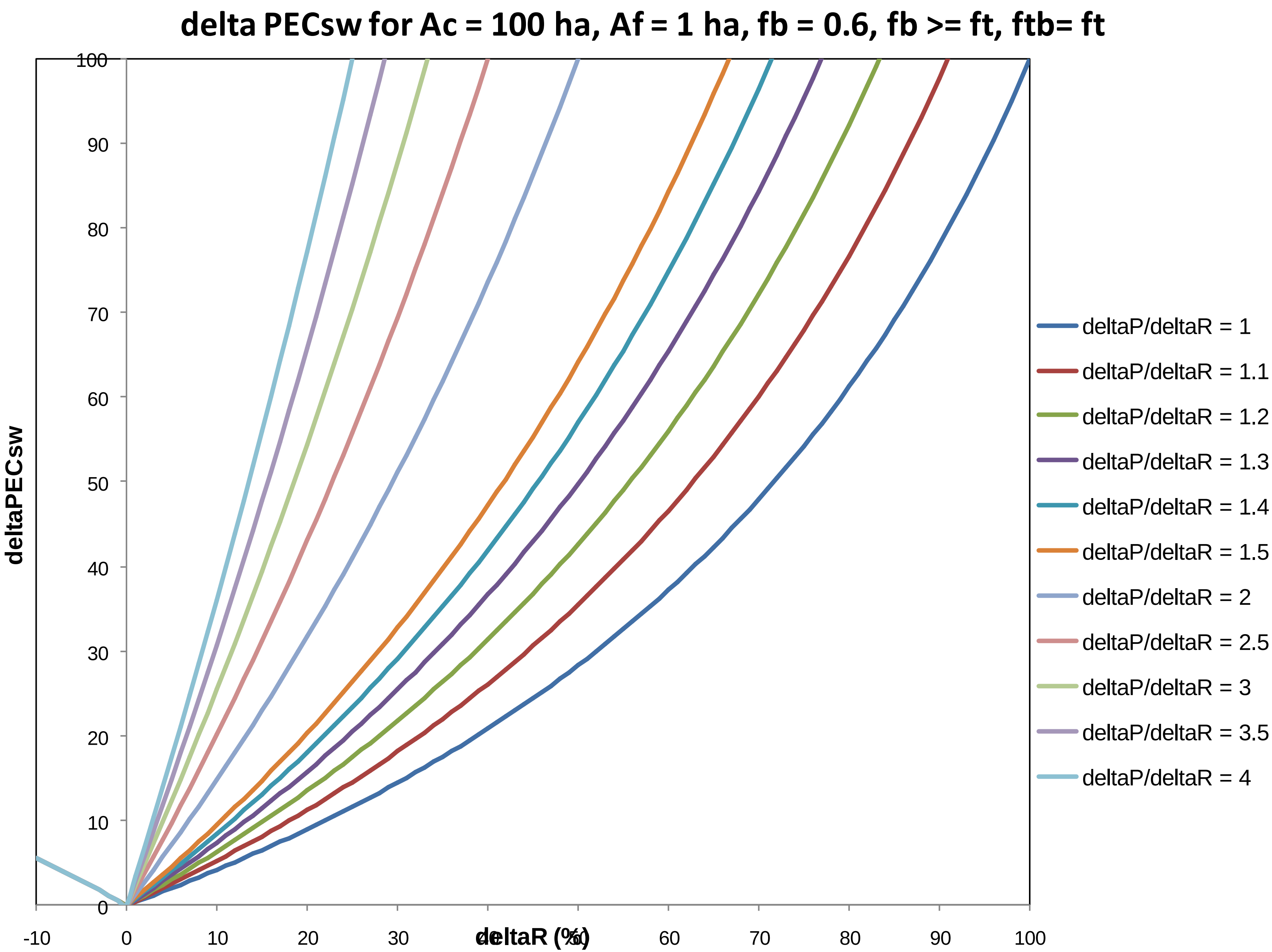
Af	area of treated field (m^2)
Ac	area of upstream catchment (m^2)
ft	fraction of upstream catchment treated with the simulated pesticide
frf	fractional reduction of pesticide runoff flux (frf = deltaP/100)
frv	fractional reduction of surface runoff volume (frv = deltaR/100)
fb	fraction of upstream catchment that is equipped with VFS (in SWAN assumed equal to ft)
ftb	fraction of upstream catchment that is treated AND equipped with VFS

- Equation is valid if ft = ftb and fb ≥ ft
- The treated area fraction ft doesn't occur in the equation any more.
- The following 4 diagrams show deltaPECsw as a function of deltaR (= frv * 100 %) for different ratios of deltaP/deltaR = frf/frv (same diagram) and different values of fb (different diagrams)

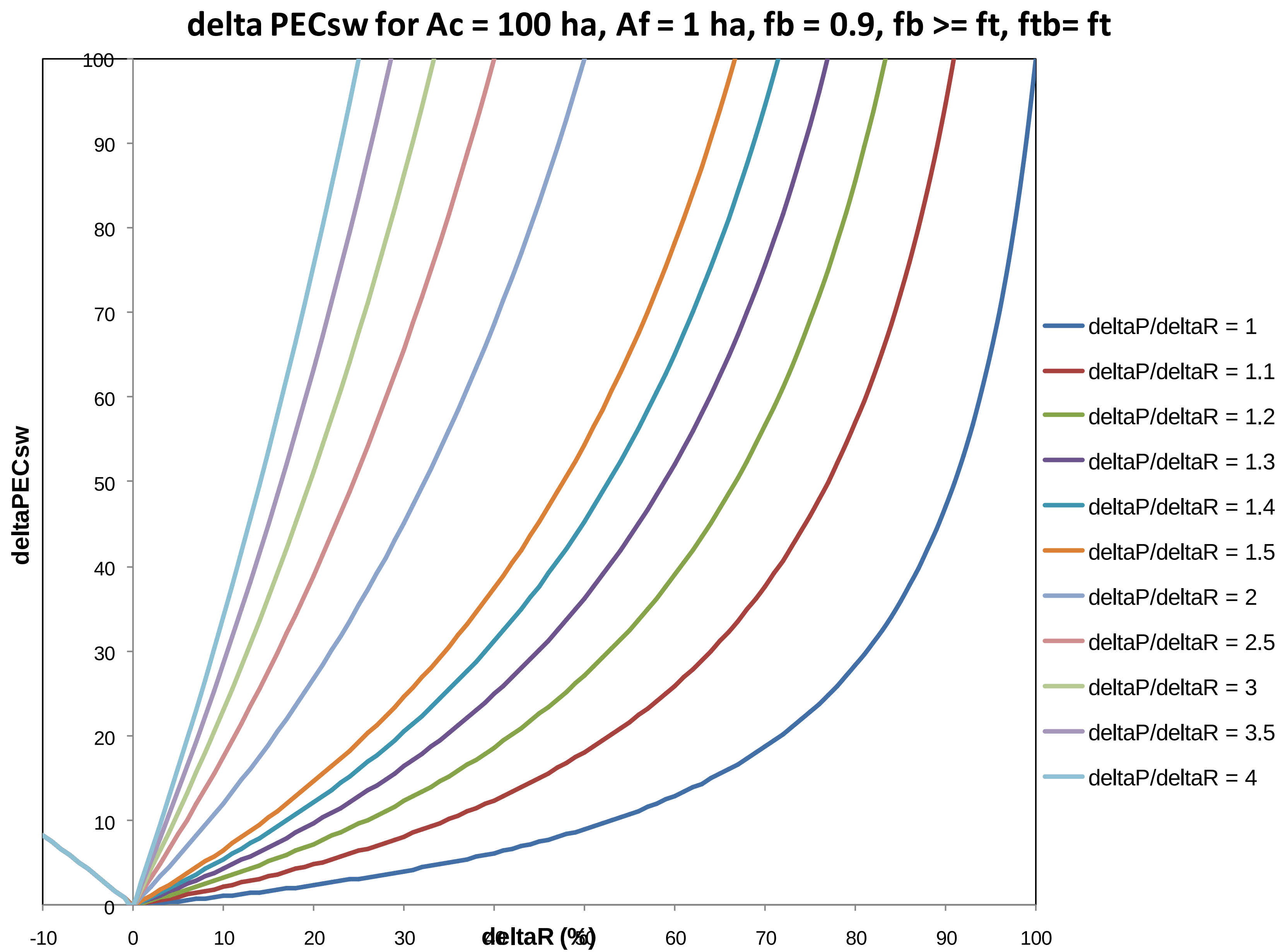
SWAN case: 20 % of UC area equipped with VFS



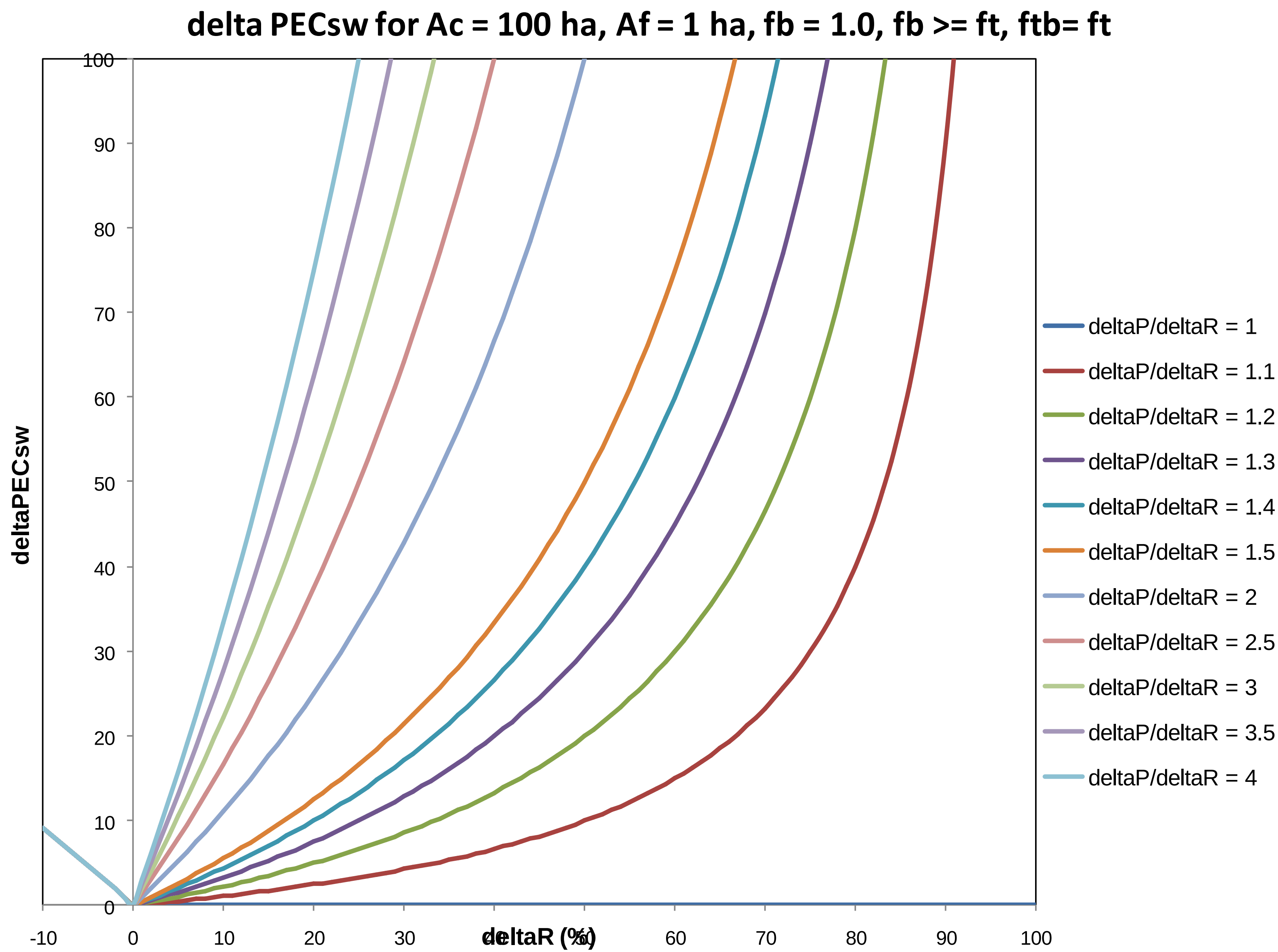
Intermediate case: 60 % of UC area equipped with VFS



Intermediate case: 90 % of UC area equipped with VFS



Extreme case: 100 % of UC area equipped with VFS



Discussion on UC fraction equipped with VFS

- In SWAN or SWAN-VFSMOD, deltaPECsw is approximately equal to deltaP (if the assumptions are met that baseflow, standing water volume and lateral inflow are small compared to the surface runoff volume).
- However, if a larger proportion of the upstream catchment is equipped with buffer strips, deltaPECsw can be a lot less than deltaP.
- In our opinion, the SWAN assumptions (fb = ft = ftb) are not meaningful for arable crops:
    1) VFS are structures with perennial vegetation. They are not installed and removed in one single season specifically for the application of a given pesticide.
    2) EU Cross Compliance and good agricultural practice require crop rotation on arable fields. Thus, in theory all arable fields in the upstream catchment can potentially be cropped with the crop to be modelled and be treated with the pesticide of concern, albeit not in the same season.

Analytical relationship for deltaPECsw (FOCUS pond)

$$deltaPECsw = (1 - \frac{(1 - frf)(Af * V + Vpo)}{Af * V(1 - frv) + Vpo}) * 100\%$$

with

Af	area of treated field (m²)
V	surface runoff volume leaving the field (PRZM output; mm)
Vpo	standing volume of the pond (L)
frf	fractional reduction of pesticide runoff flux (frf = deltaP/100)
frv	fractional reduction of surface runoff volume (frv = deltaR/100)

- In the case that VPo is >> Af*V, the solution can be approximated as deltaPECsw = deltaP
- FOCUS pond: for 20 mm surface runoff, Af*V/ Vpo = 0.1
- However, note that the equation holds only if there are no significant residual concentrations in the water column from previous runoff or spray drift input events.

3. PRZM-VFSMOD-TOXSWA modelling study

Objectives of the modelling study

1) Determine the effects of
   - the presence of a shallow water table (boundary condition + initial water table depth)
   - flow concentration
   - length of the simulation period

   on the reduction efficiencies of VFS for the FOCUS Runoff scenarios:
   - reduction efficiencies for the whole p2t time series :
     delta PECsw,max, deltaPECsed,max
   - event-based reduction efficiencies calculated by VFSMOD: deltaR, deltaQ, deltaE, deltaP

2) Establish relationships between the various deltas and potential explanatory variables:
   - PRZM output and scenario settings: PRECIP, RUNF, ESLS, wb_type, scenarionr, appmonth, txwperiod, BC, WTD, FWIDTH, VL, Koc

Modelling study: simulation design

- R + E / stream
  2 (substances) *
  4 (scenario / crop) *
  3 (application month) *
  10 (lower boundary condition of VFSMOD / water table depth) *
  5 (filter strip effective flow width) *
  4 (filter strip length in flow direction) *
  2 (length of simulation period)
  = 9600 simulation runs (PRZM-VFSMOD-TOXSWA)

- R + E / pond
  2 (substances) *
  1 (scenario / crop) *
  3 (application month) *
  10 (lower boundary condition of VFSMOD / water table depth) *
  5 (filter strip effective flow width) *
  4 (filter strip length in flow direction) *
  2 (length of simulation period)
  = 2400 simulation runs

- Crop: winter cereals for R1, R3, R4; maize for R2
- PRZM-TOXSWA control simulations (no VFS) for comparison (48 and 12, resp.)

Modelling study: fixed parameters

input variable		unit	value
name	description		
degHLsoil	degradation half-life soil	d	100
nf	Freundlich exponent nf	-	0.9
degHLwc	degradation half-life water column	d	30
degHLsed	degradation half-life sediment	d	30
foliarWC	foliar washoff coefficient	1/cm	0.5
PUF	plant uptake factor	-	0.5
vp	vapour pressure at reference temperature	mPa	1.0e-3
watersolub	water solubility at reference temperature	mg/L	100
apprate	application rate	g/ha	1000

Modelling study: varied parameters

input variable	value
lower boundary condition (lowerBC)	0 (no water table) 1 (Dupuit-Forchheimer) 2 (vertical saturated flow) 3 (simplified)
water table depth (WTD)	1 m 2 m 3 m
Filter strip effective flow width FWIDTH	equal to field outlet width 0.5 * field outlet width 0.1 * field outlet width 0.05 * field outlet width 0.01 * field outlet width
Filter strip length in flow direction VL	5 m 10 m 20 m 30 m
length of VFSMOD / TOXSWA simulation period (PRZM always simulates 20 years)	12 months 240 months
pesticide application month	March (3) June (6) October (10)

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Modelling study: execution

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- PRZM-VFSMOD-TOXSWA coupling: Footways
- Differences between our PRZM-VFSMOD-TOXSWA coupling and SWAN-VFSMOD : cf. supplementary slides
- Calculations: Footways cluster
- VFSMOD version used: vfsm.exe v. 4.2.3 from 08/2013

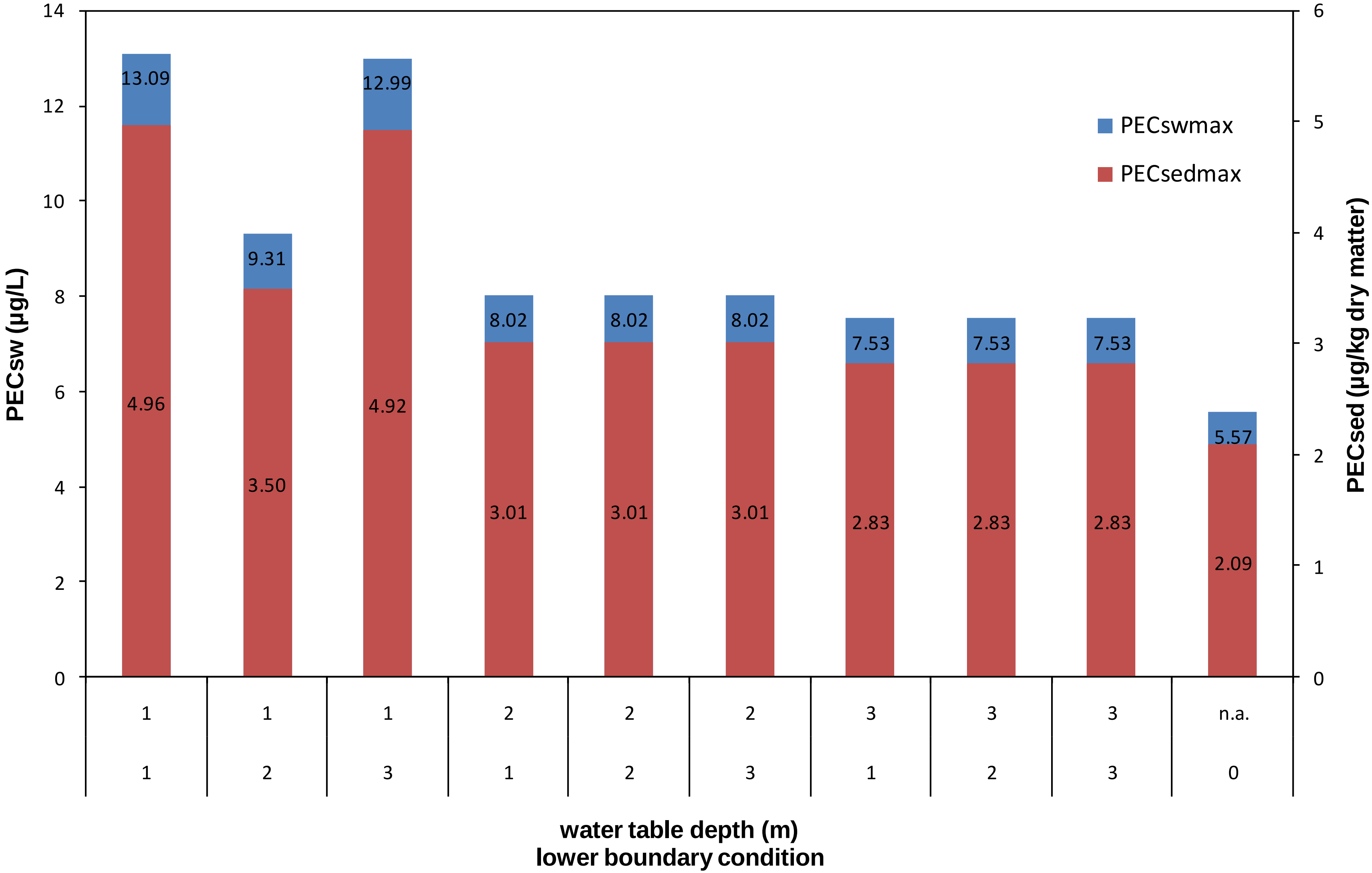
Modelling study: results (1)

- TOXSWA crashes for the stream scenarios R2, R3 und R4 if the simulation period is 240 months (numerical problems)
  → results for 240 months only for R1s and R1p
  → this confirms our decision to use STEPS instead of TOXSWA for the GERDA tool
- 12000 PRZM-VFSMOD runs with VFSMOD results for each event:
  - deltaQ
  - deltaR
  - deltaE
  - deltaP
- 8400 PRZM-VFSMOD-TOXSWA runs with TOXSWA results:
  - PECsw,max
  - PEDsed,max
  - TWACsw (1, 2, 4, 7, 14, 21, 28, 42, 50, 100 d)
  - TWACsed
- 42 PRZM-TOXSWA control simulations with TOXSWA results

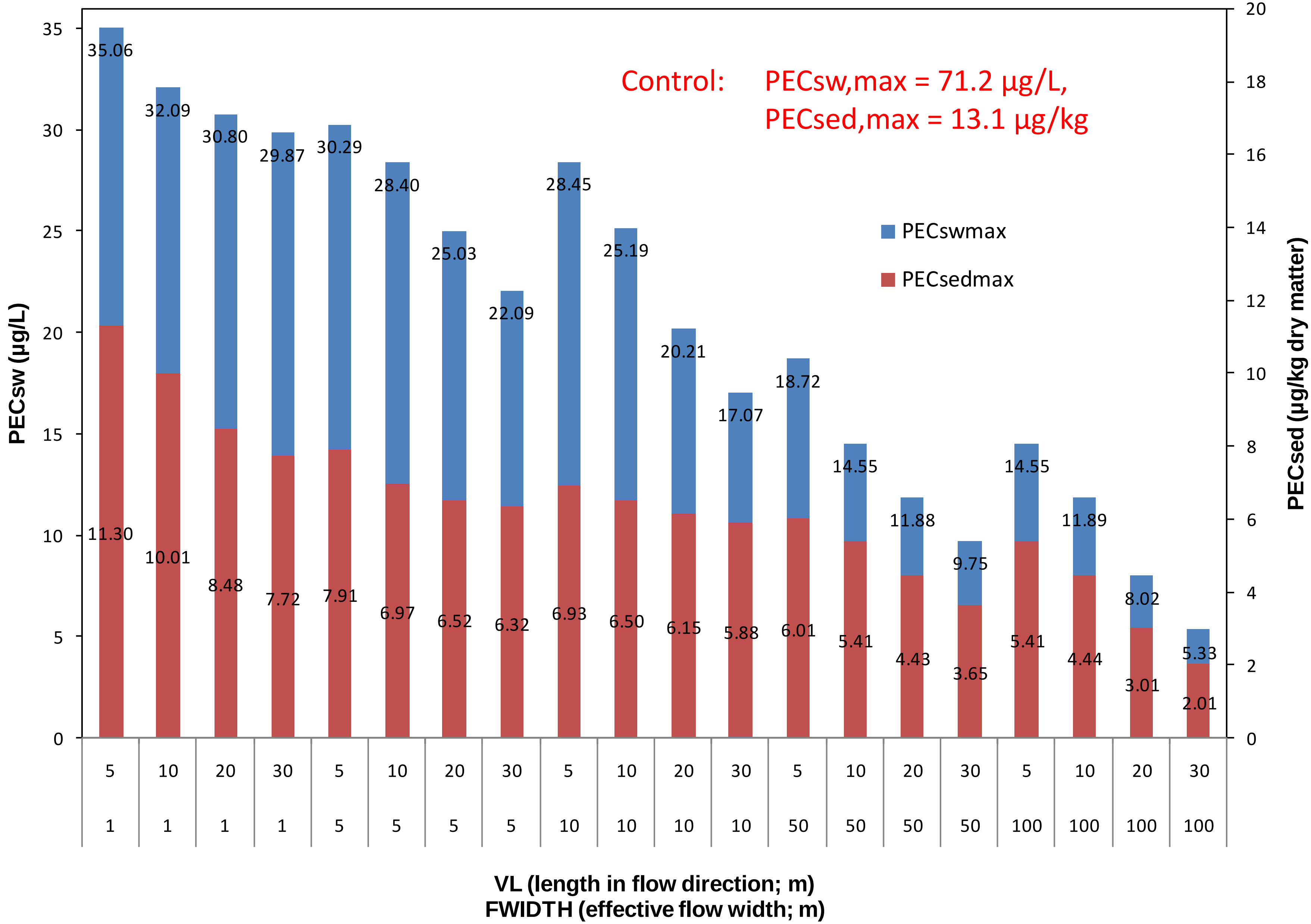
Modelling study: results (2)

- 9 independent variables → complex design with many interactions
- asymmetry in available results due to FOCUSsw scenario definition and TOXSWA crashes
- systematic evaluation necessary → MLR
- selected examples shown in the following 3 figures
  - effect of lower boundary condition (BC) and initial water table (WTD)
  - effect of VFS flow length (VL) and effective flow width (FWIDTH)

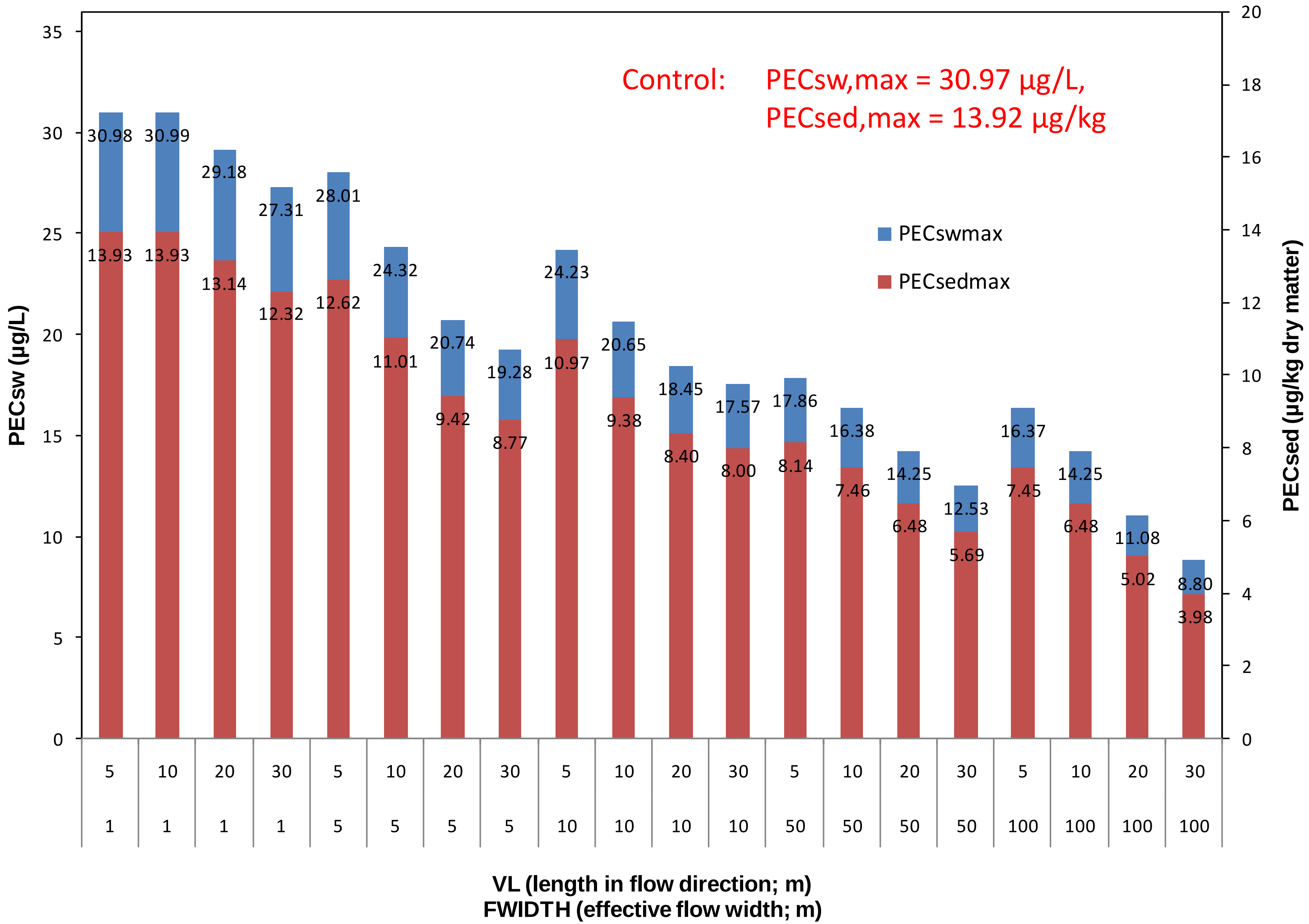
Effect of BC and WTD for: R1 stream, Koc = 100 L/kg, 240 months, appmonth = 10, VL = 20 m, FWIDTH = 100 m



Effect of VL and FWIDTH for: R1 stream, Koc = 100 L/kg, 240 months, appmonth = 10, BC = 1, WTD = 2 m



Effect of VL and FWIDTH for: R4 stream, Koc = 100 L/kg, 12 months, appmonth = 10, BC = 1, WTD = 2 m



Observations

- An effect of BC and WTD on PECsw,max / PECsed,max is mainly observed for small hydraulic loads (cf. Lauvernet et al., 2011)
- VL and FWIDTH are considerably more important than the lower boundary condition (BC) and the initial water table depth (WTD)
- PECsw,max are difficult to compare between different combinations of VL and FWIDTH, because often not the same event is responsible for the PECsw,max
- Worst-case combinations of VL and FWIDTH
  - sometimes still lead to substantial reduction of PECsw,max (cf. 2nd figure with about 50 % reduction)
  - sometimes lead to no reduction of PECsw,max at all (cf. 3rd figure)

Closer examination of one example

- Settings: VL = 5, FWIDTH = 1, R1 stream, Koc = 100, 240 months, appmonth = 10, lowerBC = 1, WTD = 2 m
- VFSMOD results for the runoff event responsible for PECsw,max:
  - deltaQ = 8.8 %
  - deltaR = 5.1 %
  - deltaE = 99.8 %
  - deltaP = 50.0 %

→ only 5 % reduction of surface runoff volume, but 50 % reduction of pesticide load (for a weakly sorbing compound where the vast majority is in the dissolved phase)

→ How reliable is the multiple regression equation of Sabbagh et al. (2009) for deltaP that is used in VFSMOD? Cf. discussion in Reichenberger and Pires (2014)

4. Multiple linear regression analysis

MLR: Materials and methods (1)

- Of the 12000 PRZM-VFSMOD simulations, only those with 240 months simulation period were used.
- Numbers of potential explanatory variables:
  - pond / no shallow water table simulated: 6 variables
  - pond / shallow water table simulated: 8 variables
  - stream / no shallow water table simulated: 9 variables
  - stream / shallow water table simulated: 11 variables
- After removing 132 failed runs and all runs where deltaQ = 100 %, the numbers of VFSMOD events remaining for the MLR were:
  - pond / no shallow water table: 33366 records
  - pond / shallow water table: 330569 records
  - stream / no shallow water table: 178212 records
  - stream / shallow water table: 1810010 records

MLR: Materials and methods (2)

- 2 types of MLR
  - linear (assuming an additive relationship independent and dependent variables)
  - log-linear (independent and dependent variables logarithmized; assuming a multiplicative relationship between independent and dependent variables)
- 4 different dependent variables: deltaQ, deltaR, deltaE, deltaP
- 10 different subsets of data
  - pond / no shallow water table
  - pond / shallow water table (BC > 0)
  - pond / shallow water table (BC = 1)
  - pond / shallow water table (BC = 2)
  - pond / shallow water table (BC = 3)
  - stream / no shallow water table
  - stream / shallow water table (BC > 0)
  - stream / shallow water table (BC = 1)
  - stream / shallow water table (BC = 2)
  - stream / shallow water table (BC = 3)

MLR: Most important variables

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Tab. 26: Most important independent variables in the multiple regression

water body	lower BC	reg. type	deltaQ	deltaE	deltaR	deltaP
			three variables with highest abs(regression coefficient)			
	0		ratio_FWIDTH_fow , Runf, Precip	ratio_FWIDTH_fow , Runf, VL	ratio_FWIDTH_fow , Runf, Precip	ratio_FWIDTH_fow, Runf, Precip
	>0		ratio_FWIDTH_fow, WTD, Runf	ratio_FWIDTH_fow , Runf, VL	ratio_FWIDTH_fow, WTD, Precip	ratio_FWIDTH_fow, Runf, WTD
pond	1	linear	ratio_FWIDTH_fow, WTD, Runf	ratio_FWIDTH_fow , Runf, VL	ratio_FWIDTH_fow, WTD, Precip	ratio_FWIDTH_fow, WTD, Runf
	2		ratio_FWIDTH_fow , Runf, Precip	ratio_FWIDTH_fow , Runf, VL	ratio_FWIDTH_fow, WTD, Precip	ratio_FWIDTH_fow, Runf, WTD
	3		ratio_FWIDTH_fow, WTD, Runf	ratio_FWIDTH_fow , Runf, VL	ratio_FWIDTH_fow, WTD, Precip	ratio_FWIDTH_fow, WTD, Runf
	0		ratio_FWIDTH_fow, VKS_cm_h, VL	ratio_FWIDTH_fow, VKS_cm_h, VL	ratio_FWIDTH_fow, VKS_cm_h, VL	ratio_FWIDTH_fow, VKS_cm_h, OCP
	>0		ratio_FWIDTH_fow, VKS_cm_h, WTD	ratio_FWIDTH_fow, VKS_cm_h, VL	ratio_FWIDTH_fow, VKS_cm_h, WTD	ratio_FWIDTH_fow, VKS_cm_h, OCP
stream	1	linear	ratio_FWIDTH_fow, WTD, Precip	ratio_FWIDTH_fow, VKS_cm_h, VL	ratio_FWIDTH_fow, VKS_cm_h, WTD	ratio_FWIDTH_fow, VKS_cm_h, OCP
	2		ratio_FWIDTH_fow, VKS_cm_h, Precip	ratio_FWIDTH_fow, VKS_cm_h, VL	ratio_FWIDTH_fow, VKS_cm_h, Precip	ratio_FWIDTH_fow, VKS_cm_h, OCP
	3		ratio_FWIDTH_fow, WTD, VKS_cm_h	ratio_FWIDTH_fow, VKS_cm_h, VL	ratio_FWIDTH_fow, VKS_cm_h, WTD	ratio_FWIDTH_fow, VKS_cm_h, OCP
	0		Runf, VL, ratio_FWIDTH_fow	VL, ratio_FWIDTH_fow, Precip	Runf, VL, ratio_FWIDTH_fow	Runf, ratio_FWIDTH_fow, VL
	>0		VL, ratio_FWIDTH_fow, Runf	Precip, VL, ratio_FWIDTH_fow	VL, ratio_FWIDTH_fow, Runf	Runf, VL, ratio_FWIDTH_fow
pond	1	loglinear	VL, ratio_FWIDTH_fow, Runf	Precip, VL, ratio_FWIDTH_fow	VL, ratio_FWIDTH_fow, Runf	Runf, VL, ratio_FWIDTH_fow
	2		VL, ratio_FWIDTH_fow, Runf	VL, Precip, ratio_FWIDTH_fow	VL, ratio_FWIDTH_fow, Runf	Runf, VL, ratio_FWIDTH_fow
	3		VL, ratio_FWIDTH_fow, Runf	Precip, VL, ratio_FWIDTH_fow	VL, ratio_FWIDTH_fow, Runf	Runf, VL, ratio_FWIDTH_fow
	0		VL, ratio_FWIDTH_fow, Runf	Precip, VL, ratio_FWIDTH_fow	VL, ratio_FWIDTH_fow, Runf	CCP, ratio_FWIDTH_fow, VL
	>0		-	-	-	-
stream	1	loglinear	VL, ratio_FWIDTH_fow, Runf	Precip, Runf, VL	VL, VKS_cm_h, ratio_FWIDTH_fow	CCP, ratio_FWIDTH_fow, VL
	2		VL, ratio_FWIDTH_fow, VKS_cm_h	Precip, VL, Runf	VKS_cm_h, VL, ratio_FWIDTH_fow	CCP, ratio_FWIDTH_fow, VL
	3		VL, ratio_FWIDTH_fow, Runf	Precip, Runf, VL	VKS_cm_h, VL, ratio_FWIDTH_fow	CCP, ratio_FWIDTH_fow, VL

MLR: Central findings

- deltaE is predicted badly by both the linear and the loglinear fit. Obviously there is neither an additive nor a multiplicative relationship between the independent variables and deltaE.
- For deltaQ, deltaR and deltaP, the loglinear fit yielded a better r^2 than the linear fit.
- Most important variables (loglinear fit):
  - Filter strip length VL always among the three most important variables
  - ratio_FWIDTH_fow (ratio of FWIDTH to "field outlet width") also almost always among the three most important variables

5. Overall conclusions

Overall conclusions (1)

- Flow concentration, in form of VFSMOD parameter FWIDTH or the derived quantity ratio_FWIDTH_fow (ratio of effective flow width to the field outlet width) is a decisive factor for the efficiency of buffer strips (deltaQ, deltaR, deltaE, deltaP). It is of similar importance as VL. Therefore, FWIDTH and ratio_FWIDTH_fow need to be chosen very carefully when setting up VFSMOD scenarios.
- The presence of a shallow water table affects VFSMOD-calculated buffer strip efficiencies less than flow concentration, but is not negligible. When a shallow water table is present, the depth of the initial water table is more important than the lower boundary condition (1, 2 or 3) itself. BC1 yields the strongest deviations from infiltration behaviour without shallow water table.
- Since deltaPECsw $\approx$ deltaP for both FOCUS stream (with the SWAN scenario assumptions) and pond, the effect of the length of the TOXSWA simulation period on deltaPECsw,max was not further investigated. However, it can be stated that TOXSWA (toxswa_focus.exe from 2009) is not able to simulate 20 years for the R2, R3 and R4 stream scenarios.

Overall conclusions (2)

- A multiple regression analysis for VFSMOD output variables (deltaQ, deltaR, deltaE, deltaP) with PRZM output and VFSMOD scenario settings as independent variables didn't yield relationships of sufficient quality, but permitted to identify the most important variables.

- Finally: To obtain meaningful results of step 4 surface runoff simulations, it is not sufficient to get only the VFSMOD modelling right. The scenario assumptions outside VFSMOD (notably fb) must be realistic as well.

Thank you for your attention!

Vielen Dank für Ihre Aufmerksamkeit!

Merci pour votre attention!

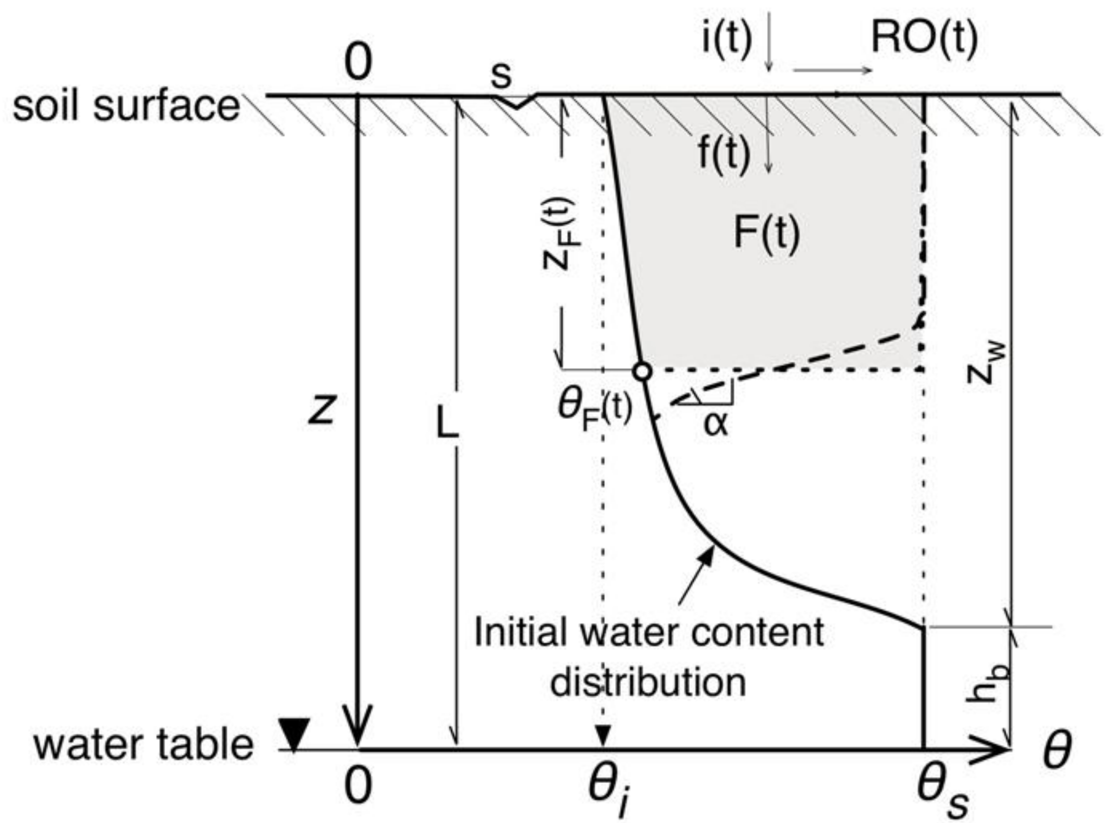
Supplementary slides

Discussion on UC fraction equipped with VFS (2)

- Given that in FOCUS step 3 the hydrological signal of the UC is identical to the hydrological signal of the 1 ha field, it is likely that the whole FOCUS UC is supposed to have the same land use as the field.
- Possible solutions for the parameterization of the upstream catchment:
  a) The whole upstream catchment is arable and equipped with VFS (fb = 1). This is possibly a little too worst-case for the PECsw calculation.
  b) Only part of the upstream catchment is arable, and only the arable part is equipped with VFS. However, then the non-arable part (e.g. pasture, meadows or forest) should produce less (and less frequently) surface runoff than the arable part. This would considerably complicate the calculations of water fluxes in the modified p2t file.
  c) A compromise is found: The whole upstream catchment is considered as arable, and fb is set to a reasonable and realistic value > 0.2 and < 1. For instance, fb = 0.6 would imply that out of the area not treated with the pesticide of concern, one half is equipped with buffer strips and the other half is not. → Solution adopted for GERDA.

Infiltration and redistribution in VFSMOD before water table is reached

- At the beginning of the event, the soil above the shallow water table is in hydrostatic equilibrium with the shallow water table.
- The wetting front proceeds from the surface (according to Green-Ampt) and fills up the profile from the top.
- Once the wetting front reaches the upper boundary of the capillary fringe (t = tw), the profile is completely saturated and the boundary condition changes.



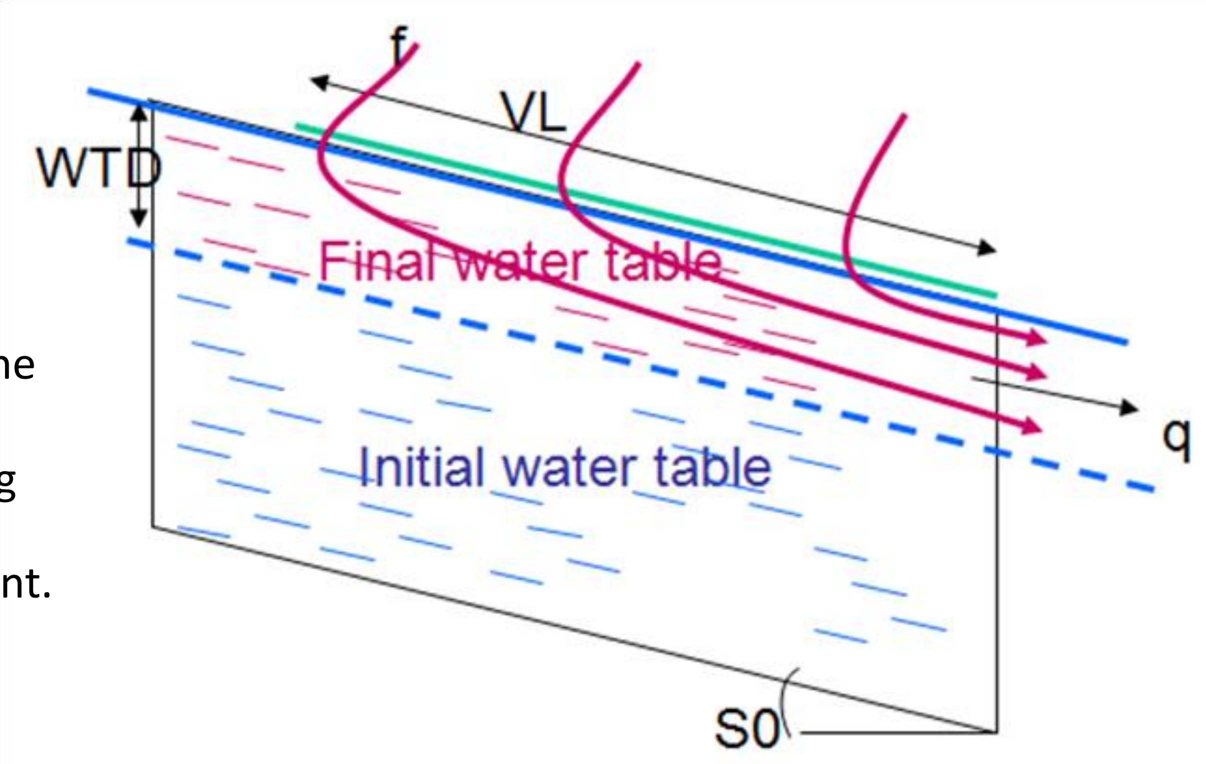
Source: Rafael Muñoz-Carpena

Water flow in VFSMOD for BC1 once profile is saturated

- For t ≥ tw the initial water table is a no-flux boundary condition (due to a zero hydraulic gradient).
- Infiltration flow at the surface (Q_f) is only allowed by lateral flow (Q_L) at the downslope boundary of the simulated soil elementary volume.

Dupuit-Forchheimer assumptions:

- The flow is horizontal at any vertical cross-section.
- The velocity is constant over the depth.
- The velocity is calculated using the slope of the free water surface as the hydraulic gradient.
- The slope of the water table is relatively small.



Source: N. Carluer, provided by Rafael Muñoz-Carpena

Differences between our PRZM-VFSMOD-TOXSWA coupling and SWAN-VFSMOD (1)

Item	SWAN-VFSMOD	PRZM-VSFMOD-TOXSWA UBA	remarks
length of simulation period	fixed to 12 months	flexible (12 or 240 months)	
incoming flow sediment concentration CI	bug: underestimated by a factor of 2.2 (unit error)	correct calculation	the bug was related to misinterpretation of the unit of the column “erosion mass” in the p2t file, which is kg/h and not kg/(ha*h)
field dimensions for pond	SWIDTH = 100 m, SLENGTH = 100 m (i.e. same value as for stream)	SWIDTH = 60 m, SLENGTH = 75 m	The source area is calculated by VFSMOD internally as SWIDTH * SLENGTH. Hence, SWIDTH * SLENGTH must yield 0.45 ha to match the FOCUSsw pond scenario definition. The geometry of the field (which constitutes the source area) is complicated for the FOCUS pond, the field is not square and is arranged around the pond. Anyway, we assumed SWIDTH = 60 m and SLENGTH = 75 m to match the source area of 0.45 ha.

Differences between our PRZM-VFSMOD-TOXSWA coupling and SWAN-VFSMOD (2)

Item	SWAN-VFSMOD	PRZM-VSFMOD-TOXSWA UBA	remarks
FWIDTH for pond	100 m (i.e. same value as for stream)	30 m (base value in the absence of runoff concentration)	The length of the strip contributing erosion inputs is set to 30 m in FOCUSsw for the pond. Hence, we set field_outlet_width (not a VFSMOD parameter; defined as “length of the field boundary through which surface runoff and eroded sediment leave the field) to 30 m as well. Consequently, the base value of FWIDTH (no runoff concentration) equals 30 m as well.
possibility to simulate runoff concentration	no	yes	FWIDTH is not changeable in SWAN-VFSMOD

Differences between our PRZM-VFSMOD-TOXSWA coupling and SWAN-VFSMOD (3)

Item	SWAN-VFSMOD	PRZM-VSFMOD-TOXSWA UBA	remarks
runoff hydrograph	rectangular	triangular	Rafael Muñoz-Carpena recommends a triangular hydgrograph to avoid numerical problems (kinematic shock); cf. technical note Tech_Note_Field_Hydrograph_VFSMOD.pdf
shallow water table	absent	absent or present (three different lower BC for water table)	If a shallow water table is to be modelled, VFSMOD requires additional parameters (Van Genuchten alpha, N, m). These have been calculated with the HYPRES ptfs according to Woesten et al. (1998) from the VFS soil properties in Brown et al. (2012)

MLR: Rationale

- The idea was to establish multiple regression equations for different dependent variables and different sets of independent variables.
- However, for the FOCUS stream (with SWAN scenario assumptions) and for the FOCUS pond deltaPECsw $\approx$ deltaP.
  - Hence, instead of performing a regression for deltaPECsw,max it is sufficient to perform a regression for the VFSMOD output deltaP.
  - This, in turn, makes it unnecessary to restrict oneself only to the runoff events responsible for the global PECsw,max in TOXSWA. Instead, one can analyze all surface runoff events simulated by VFSMOD.
- deltaP is a known function of deltaQ and deltaE (the multiple regression equation by Sabbagh et al. (2009) that is implemented in VFSMOD). Nevertheless, we decided to do the regression analysis for all four VFSMOD output variables deltaP, deltaQ, deltaE and deltaR.

MLR: Results

- For each of the 19 successful combinations of subset and type of fit, three output files were generated:
  - 1 .pdf with 4 scatter plots of fitted values vs. “measured” values (i.e. values calculated by VFSMOD)
  - 1 .txt with a summary of the 4 regressions (variables used + regression outputs)
  - 1 .Rout with an echo of the commands executed by R
- All results are available upon request in a .rar archive.

MLR: Goodness of fit

- deltaE is predicted badly by both the linear and the loglinear fit. Obviously there is neither an additive nor a multiplicative relationship between the independent variables and deltaE.
- For deltaQ, deltaR and deltaP, the loglinear fit yielded a better r^2 than the linear fit.
- For the loglinear fit, r^2 is better for deltaP than for deltaQ or deltaE, although VFSMOD calculates deltaP as a function of deltaQ and deltaE.
- There were more scatter and more outliers for the BCs with a shallow water table than for the BC without a water table. This can probably be explained by the fact that in shallow water table simulations with VFSMOD, a switch of boundary conditions occurs when the wetting front reaches the capillary fringe.
- In terms of statistical and visual goodness-of-fit, there is a slight decrease in the order BC 0 > BC 2 > BC 3 > BC 1 (i.e. in the order of increasing hydrologic complexity and change in infiltration rate at the switching point).

MLR: Most important variables (loglinear fit)

- Filter strip length VL always among the three most important variables
- ratio_FWIDTH_fow (ratio of FWIDTH to "field outlet width") also almost always among the three most important variables
- Pond:
  - for deltaQ, deltaR and deltaP always the same three most important variables: Runf, ratio_FWIDTH_fow and VL.
  - for deltaE, it's Precip, ratio_FWIDTH_fow and VL
  - the lower boundary condition changes only the order of the three variables, but not their presence
- Stream:
  - for deltaP always the same three most important variables, in the same order: the scenario-specific variable CCP is first, followed by ratio_FWIDTH_fow and VL
  - for deltaQ and deltaR, VL and ratio_FWIDTH_fow always among the three most important variables
  - further important variables: Runf for deltaQ, and the scenario-specific variable VKS_cm_h for deltaR and less so for deltaQ (in 3rd position for BC2, otherwise in 4th position)
  - for deltaE, Precip and VL are always among the most important three variables

Conclusion on the equation of Sabbagh et al. (2009)

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- The regression equation of Sabbagh et al. (2009) doesn't seem to be fundamentally flawed.
- It seems usable for the purpose of regulatory risk assessment in the tool GERDA, especially in view of the fact that at the moment there is no alternative calculation method for deltaP available.
- However, further research is suggested:
  - investigate the range of the applicability of the equation using both additional experimental validation data points and VFSMOD outputs of deltaQ and deltaE
  - redo the regression analysis
    - using the original calibration datasets with correctly treated data points
    - using additional experimental data points for calibration and validation
    - experimenting with alternative structures of the equation

References (1)

Lauvernet C, Muñoz-Carpena R, Carluer N (2011). Evaluation of a mechanistic algorithm to calculate the influence of a shallow water table on hydrology sediment and pesticide transport through vegetative filter strips by sensitivity analysis. XIV Symposium Pesticide Chemistry, Piacenza, 30/08 – 01/09/2011; poster presentation

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Perez-Ovilla O (2010). Modeling runoff pollutant dynamics through vegetative filter strips: a flexible numerical approach. PhD thesis, University of Florida, Gainesville, FL, USA. 195 p.

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Mitigation options in GERDA

Spray drift mitigation:

- specify reduction efficiency of drift-reducing technology
- enter minimum distance (width of no-spray buffer) between treated area and surface water body

Surface runoff and erosion mitigation:

- Simulation of grassed buffer strips (vegetated filter strips, VFS) using VFSMOD 4.2.4
- This version of VFSMOD is able to simulate a shallow water table → parameterisation of lower boundary condition and initial water table depth (WTD) according to site hydrology, climate and season
- VFSMOD simulations are done separately for stream and ditch scenarios
- Two parameters to be entered by the GERDA user
  - VL: length of the VFS in flow direction ("buffer width")
  - FWIDTH: effective flow width of the VFS, perpendicular to the slope (allows accounting for flow concentration)
- Upstream Catchment definition: fraction of stream UC equipped with VFS (fb) set to 0.6 instead of 0.2 in SWAN

→ GERDA allows more realistic buffer strip simulations than SWAN (water table, FWIDTH, fb)