Sarajevo 21 September 2016

The Environmental Fate of Pesticides

EXPOSURE ASSESSMENT

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ICPS – International Centre for Pesticides and health risk prevention

Predicted environmental concentrations (PECs)

- To estimate such concentrations in perspective risk assessment, predictive models are used
- Models currently accepted for EU registration of PPP are derived from the work of FOCUS group, i.e. the FOrum for Co-ordination of pesticide fate models and their Use.
- Models are available for each environmental compartment.

FOCUS groups

FOrum for the Co-ordination of pesticides fate models and their USe

The work of the FOCUS groups is concerned with providing the tools for estimating environmental concentrations of a.s. for the purpose of their evaluation for inclusion in Annex I.

FOCUS

FOrum for the Co-ordination of pesticides fate models and their USe

The FOCUS organisation:

- steering committee
- working groups.

Working groups. Experts from:

- regulatory authorities,
- industry
- research institutes.

FOCUS

- Guidance was firstly developed for leaching to groundwater (FOCUS, 1995) and later for soil persistence and surface water (FOCUS 1996 & 1997).
- The guidance developed by the workgroups included a description of the relevant models and their strengths and weaknesses. Any PEC model calculation assumes a scenario which is therefore an important element of the guidance.

FOCUS

The FOCUS Steering Committee prescribed that about 10 realistic worst case scenarios should be developed, and that input files for these scenarios should be developed

FOCUS RESULTS

Identified proper model for PEC calculation:

- **Groundwater** → 4 models
- **Surface water** → 1 model run-off, 1 drainage, 1 biological degradation

Identified standard scenarios for:

- **Groundwater** → 9 European scenarios
- **Surface water** → 10 European scenarios

FOCUS models

- **Soil**
  - A very simple equation is used to estimate initial concentration
  - 4 different kinetics are used to estimate dissipation of active ingredients over time (SFO, FOMC, DFOP, HS)
  - Excel spreadsheet
- **Groundwater**
  - PELMO
  - PEARL
  - MACRO
  - PRZM
- **Surface water**
  - Steps 1-2
  - SWASH package (MACRO, PRZM, TOXSWA) – Step3
  - SWAN (mitigation measures) – Step 4
- **Air**
  - Different models are available (e.g. EVA 2.0) for estimating short and long-range transport (rarely used in dossiers)

http://esdac.jrc.ec.europa.eu/projects/focus-dg-sante

JOINT RESEARCH CENTRE

EUROPEAN SOIL DATA CENTRE (ESDAC)

SDAC > PROJECTS > FOCUS DG SANTE

About ESDAC

Events

FOCUS DG SANTE

Welcome to the home page of FOCUS DG SANTE, i.e. the FOrum for Co-ordination of pesticide fate models and their USe. From this site you can c currently approved versions of FOCUS simulation models and FOCUS scenarios, that are used to calculate the concentrations of plant protection groundwater and surface water in the EU review process according to Regulation (EC) No 1107/2009. Furthermore this site contains links to the r FOCUS workgroups.

This website is refered to by the EC website on Food Safety under "Guidelines on Active Substances and Plant Protection Products" - Fate and Bel

- Overview of FOCUS DG SANTE
- Version Control
- Documentation
- FOCUS Notice Board
- What is new in Focus

…In practice…
How to calculate PEC?

SOIL PEC

Which information is needed to calculate PECsoil?

- **Application details** (retrievable from GAP)
  - Rate
  - Number of applications
  - Crop(s)
  - If multiple applications are needed: interval between applications
- **Crop interception** (relative to crop type and BBCH scale)
- **Degradation details**
  - DT_{50} from soil degradation studies

PEC soil calculation

1st tier: DT_{50} (worst case) from lab studies

Next tiers:

- Worst-case dissipation DT_{50} from field studies (no normalisation is required)

Worst-case conditions to be selected:

✓ minimal interval between applications

✓max AR,

✓DT50 worst-case,

✓ lower foliar intercept (according to BBCH reported in the GAP table).

Crop interception

Table 1.5: Interception by other crops dependent on growth stage

Crop	Bare – emergence	Leaf development	Stem elongation		Flowering		Senescence Ripening
	BBCH#						
	0– 09	10–19	20–39		40–89		90–99
Beans (field + vegetable)	0	25	40		70		80
Cabbage	0	25	40		70		90
Carrots	0	25	60		80		80
Cotton	0	30	60		75		90
Grass##	0	40	60		90		90
Linseed	0	30	60		70		90
Maize	0	25	50		75		90
Oil seed rape (summer)	0	40	80		80		90
Oil seed rape (winter)	0	40	80		80		90
Onions	0	10	25		40		60
Peas	0	35	55		85		85
Potatoes	0	15	60		85		50
Soybean	0	35	55		85		65
Spring cereals	0	0	BBCH 20–29*	BBCH 30–39*	BBCH 40–69	BBCH 70–89	80–
			20	80	90	80	
Strawberries	0	30	50		60		60
Sugar beets	0	20	70 (rosette)		90		90
Sunflower	0	20	50		75		90
Tobacco	0	50	70		90		90
Tomatoes	0	50	70		80		50
Winter cereals	0	0	BBCH 20–29*	BBCH 30–39*	BBCH 40–69	BBCH 70–89	80
			20	80	90	80	

#The BBCH code is indicative (Meier, 2001).
##A value of 90 is used for applications to established turf.
*BBCH code of 20–29 for tillering and 30–39 for elongation.

DT_{50} normalisation

Temperature normalisation:
the temperature dependence of the degradation rate coefficient of pesticides in soil is usually described by the **Arrhenius relationship**.

$$DT_{50,T1} = DT_{50,Tref} \exp\left[\frac{E_a}{R}\left(\frac{1}{T_{ref}} - \frac{1}{T_1}\right)\right]$$

or

$$DT_{50,Tref} = DT_{50,Tact} \cdot Q_{10}^{\frac{T_{act}-T_{ref}}{10}}$$

Moisture normalisation:
Soil moisture should be normalised to pF2 (water holding capacity at 10 kPa). Values of WHC at pF2 are soil-specific. If missing, use default values for specific texture.
Normalisation follow the **Walker equation**.

$$DT_{50,norm} = DT_{50} \cdot f_{moisture}$$

$$f_{moisture} = \left(\frac{\theta_{act}}{\theta_{ref}}\right)^{0.7}$$

$$f_{moisture} = 1$$

For $\theta_{act} \geq \theta_{ref}$

Metabolites

PECs will be calculated by considering a fake direct application of the metabolite

$$AppRate_{met} = AppRate_{par} \cdot MaxObserved(\%)_{met} \cdot \frac{MolWeight_{met}}{MolWeight_{par}}$$

Using Formation fraction instead of MaxObserved will result in a further overestimation of the initial PEC.

What metabolites?

Evaluation is required for metabolites of which the concentration in the soil at any point in time is >10% (of AR), or at 2 subsequent points in time >5% (of AR)

AR = Applied radioactivity

Calculation of Predicted Environmental Concentrations in Soil

General assumptions:

- Uniform distribution of the AS in the upper soil layer
  - 5 cm depth ($PEC_{soil,max}$, $PEC_{soil,act}$, and$PEC_{soil,twa}$)
  - 20 cm depth if the AS tends to accumulate in soil ($PEC_{soil,accu}$)
    - → DT50 > 100 d and/or DT90 > 365 d
- Dry bulk density: 1.5 g/cm^3

Calculation of the global maximum PECsoil following single application

$$PEC_{soil,max} = \frac{A \cdot (1 - f_{int})}{100 \cdot d \cdot bd_{soil}}$$

$PEC_{soil,max}$	maximum concentration in soil	[mg kg^{-1}]
A_i	application rate	[g a.s. ha^{-1}]
$f_{int,i}$	fraction intercepted by plant cover	[-]
d	depth of soil layer (5 cm)	[cm]
bd_{soil}	soil bulk density (1.5 g cm^{-3})	[g cm^{-3}]

Calculation of the global maximum PECsoil following multiple applications

$$PEC_{soil,max} = \sum_{i=1}^{n} \left[\left(\frac{A_i \cdot (1 - f_{int,i})}{100 \cdot d \cdot bd_{soil}} \right) \cdot e^{-k(t_n - t_i)} \right]$$

$PEC_{soil,max}$	maximum concentration in soil after n applications	[mg kg^{-1}]
n	number of applications	[-]
A_i	application rate at i-th application	[g a.s. ha^{-1}]
$f_{int,i}$	fraction intercepted by plant cover at i-th application	[-]
d	depth of soil layer (5 cm)	[cm]
bd_{soil}	soil bulk density (1.5 g cm^{-3})	[g cm^{-3}]
k	degradation rate (= ln (2) / DT_{50})	[d^{-1}]
t_i	time of i-th application	[d]
t_n	time of n-th (last) application	[d]

Accumulation in soil

If on the basis of soil dissipation studies it is established that DT90field > 1 year the possibility of accumulation of residues in soil and the level at which a plateau concentration.

Calculation of the PECsoil,accu

- Considers the use of an AS for many years (10, 20 or 30)
- Requires the plateau concentration (PECsoil,plateau) of the AS at steady state
- The PECsoil,plateau is defined as the level of residues in soil after the winter regeneration period immediately before the first seasonal application
- The PECsoil,plateau refers soil layer depth of 20 cm (arable crops) or 10 cm (permanent crops) as a result of substance distribution in the top soil after soil cultivation over many years

Calculation of PECsoil,plateau

$$PEC_{soil,plateau} = \frac{PEC_{soil,ini}}{1 - e^{-kt}} \cdot e^{-k \cdot (t-i)}$$

$PEC_{soil,,plateau}$	plateau concentration at steady state	[mg kg^{-1}]
$PEC_{soil,ini}$	initial soil concentration following last application considering a mixing depth of 20 cm	[mg kg^{-1}]
t	interval between application seasons (365 days)	[d]
i	interval between first application and last application in the cropping season	[d]
k	degradation rate (= ln(2) / DT50)	[d^{-1}]

Calculation of PECsoil,accu

- The PECsoil,accu represents the highest potential soil concentration considering the multi-year accumulation load as background concentration plus the maximum concentration (PECsoil,max) after application in the top soil layer.

- For this purpose, the PECsoil,plateau and the PECsoil,max in the top soil layer are added

$$PEC_{soil,accu} = PEC_{soil,plateau} + PEC_{soil,max}$$

$PEC_{soil,accu}$	maximum concentration in soil for the accumulation risk assessment	[mg kg^{-1}]
$PEC_{soil,plateau}$	concentration at steady state (plateau concentration) related to the plough layer depth (e.g. 20 cm)	[mg kg^{-1}]
$PEC_{soil,max}$	maximum concentration with respect to the soil load after one application period related to a soil layer depth of 5 cm	[mg kg^{-1}]

PEC soil calculation

- How: excel spreadsheet

..\FATE TOOLS\PECsoil calculator.xls

PEC groundwater calculation

EXPOSURE: GROUNDWATER

DIRECT CONTAMINATION: wells and well borings
LEACHING: after rain events or irrigation practices.
Gravity is the main force involved.

Crucial properties of pesticides with respect to groundwater

Biodegradability → **long half-life** in soil,
Mobility → **low affinity to organic matter**
water solubility → **high water solubility**

PARAMETERS INFLUENCING CHEMICAL LEACHING TO GROUNDWATER

Physico-chemical properties of a.i. →
- sorption constant (K_{OC})
- degradation rate (DT_{50})

Soil properties →
- OM, pH, CEC, BD
- clay, sand and loam content

Climate →
- T°C, precipitation, rel. humidity

Practice →
- dose
- frequency of applications
- animal treated
- crop and crop rotation mode
- ………………..

Centro Internazionale per gli Antiparassitari e la Prevenzione Sanitaria

Ospedale Luigi Sacco POLO UNIVERSITARIO

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Parameters selection for PECgw modelling

MANAGEMENT RELATED TO SUBSTANCE/CROP PARAMETERS (REFER TO GAP)

NUMBER OF APPLICATIONS: worst case options should be used.

APPLICATION RATES: worst case options should be used. For all models, the dose should be corrected for the amount of crop interception occurring.

APPLICATION DATES: worst case options should be used, but realistic values may be used for additional simulations.

INCORPORATION DEPTH: the majority of applications are likely to be to foliage or to soil surface, and the depth is therefore unnecessary. However, some compounds may be incorporated and in such cases the label recommendation for incorporation depth (usually ca. 20 cm) should be used as input.

FOCUS

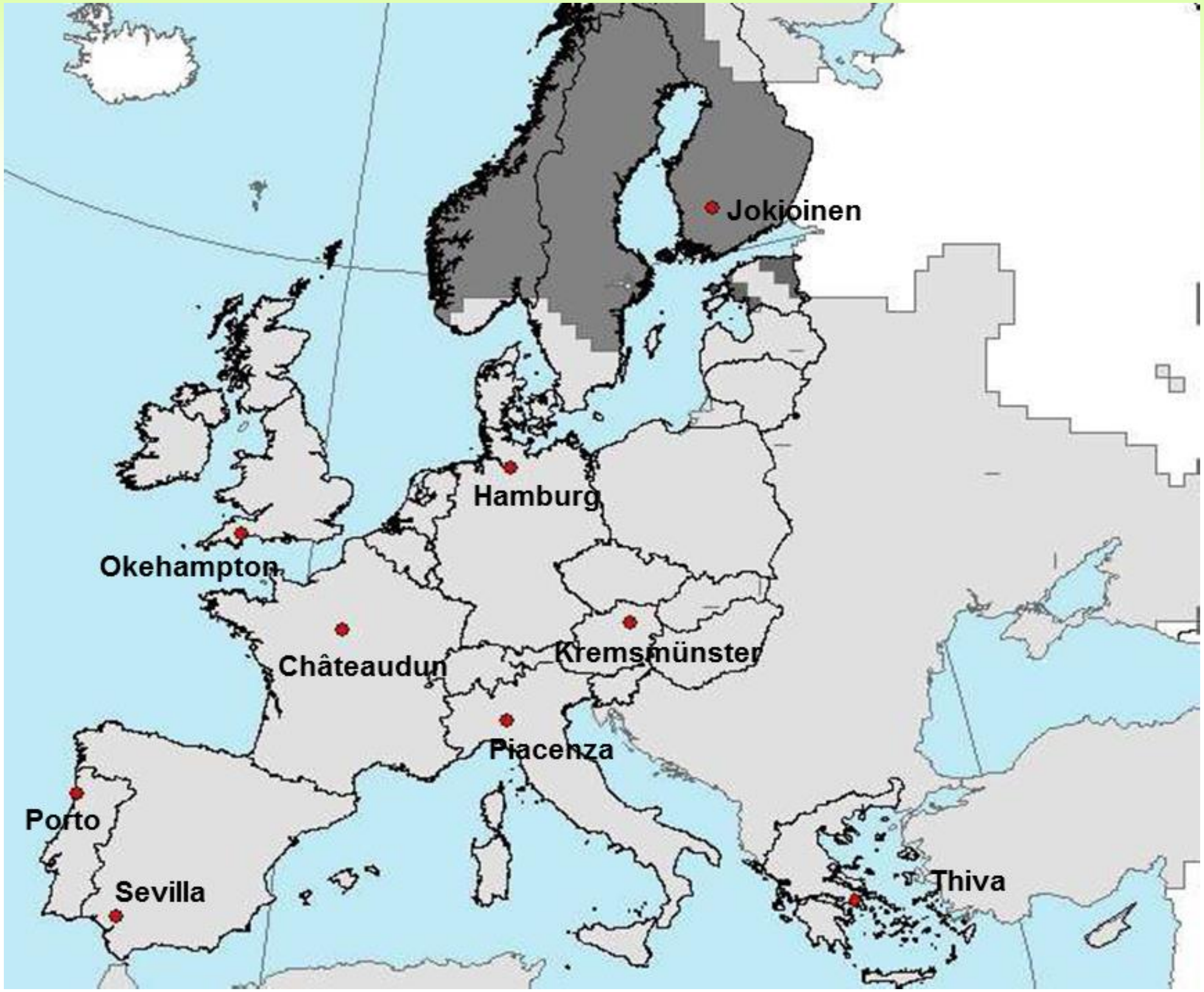
Identified proper model for PEC calculation:

Groundwater → 4 models **Pearl, Pelmo, Macro, PRZM**

Identified standard scenarios for:

Groundwater → 9 European scenarios

FOCUS scenarios



FOCUS scenarios

Crop	C	H	J	K	N	P	O	S	T
apples	+	+	+	+	+	+	+	+	+
grass (+ alfalfa)	+	+	+	+	+	+	+	+	+
potatoes	+	+	+	+	+	+	+	+	+
sugar beets	+	+	+	+	+	+	+	+	+
winter cereals	+	+	+	+	+	+	+	+	+
beans (field)		+		+	+				
beans (vegetables)							+		+
bush berries			+						
cabbage	+	+	+	+			+	+	+
carrots	+	+	+	+			+		+
citrus						+	+	+	+
cotton								+	+
linseed					+				
maize	+	+		+	+	+	+	+	+
oilseed rape (summer)			+		+		+		
oilseed rape (winter)	+	+		+	+	+	+		
onions	+	+	+	+			+		+
peas (animals)	+	+	+		+				
soybean						+			
spring cereals	+	+	+	+	+		+		
strawberries		+	+	+				+	
sunflower						+		+	
tobacco						+			+
tomatoes	+					+	+	+	+
vines	+	+		+		+	+	+	+

C Châteaudun, H Hamburg, J Jokioinen, K Kremsmünster, N Okehampton, P Piacenza, O Porto, S Sevilla, T Thiva.

…trigger values for groundwater

- **Active ingredient : 0.1 µg/L**

  refined assessment with prejudice is required, or monitoring programme of 5 y at least

- **NON-relevant metabolite : 0.75 µg/L**

  if 0.75 µg/L > NON-rel. metabolite > 10 µg/L → monitoring programme of 3 y is required **(Italy)**

  if NON-relevant metabolite is > 10 µg/L →no authorisation shall be granted

- **RELEVANT metabolite: 0.1 µg/L**

  refined assessment is required with prejudice

Parameters selection for PECgw modelling

1) Proportion of each metabolite formed or individual rate constants for the formation of each metabolite

2) Physico-chemical properties

3) Crop-management parameters taken from the intended GAP (intercept, etc.)

4) Soil sorption values (Koc, Kom)

5) Degradation rates

Parameters selection for PECgw modelling

SORPTION PARAMETERS

Koc is the Soil Organic Carbon-Water Partitioning Coefficient

$$K_{oc} = K_d / f_{oc}$$

Where $K_d = C_{solid} / C_{water}$ is the "distribution coefficient" or "soil-water" partitioning coefficient

f_{oc} = fraction of organic carbon in soil or sediment

K_{OC} values are useful in predicting the mobility of organic soil contaminants; higher K_{OC} values correlate to less mobile organic chemicals, while lower K_{OC} values correlate to more mobile organic chemicals

MOBILITÀ NEL SUOLO	K_{OC}
Molto grande	0-50
Grande	50-150
Media	150-500
Bassa	500-2000
Molo bassa	2000-5000
Immobile	>5000

Parameters selection for PECgw modelling

SORPTION PARAMETERS

PEARL, PELMO, PRZM, and MACRO now all use the **Freundlich adsorption coefficient (Kf)**, however previous versions of PRZM used the Kd. The Freundlich adsorption coefficient (Kf), is defined as:

$$x/m = Kf\ C^{1/n}$$

Freundlich adsorption isotherm

Where x/m is the content of substance sorbed (mg/kg), C is the concentration in the liquid phase (mg/L), **1/n is the exponent of the isotherm**

1/n is determined in each laboratory sorption experiment (batch sorption), and the arithmetic mean value should be used as model input.

When there is no data, a default value of 0.9 should be used.

If a linear sorption has been determined the value may be set to 1.

Parameters selection for PECgw modelling

SORPTION PARAMETERS

Regulation (EC) no 1107/2009 recommends that Soil sorption results (Kfoc, Koc or Kfom, Kom) are required from 4 SOILS FOR PARENT COMPOUND, and from 3 SOILS FOR METABOLITES

- **Where these are all agricultural soils, FOCUS recommends to use the geometric mean values of sorption constants, unless the sorption is known to be pH-dependent.**

- **If results are less than the recommended No of agricultural soils, use of worst case results (LOWEST SORPTION) is more appropriate.**

- **In cases where a large number of additional data points are available (9 or more), a median value may be more appropriate.**

Parameters selection for PECgw modelling

DEGRADATION RATES

Regulation (EC) no 1107/2009 recommends that degradation rate studies are undertaken in 4 soils for the parent compound and 3 soils for metabolites (laboratory studies initially, and then, if necessary, field studies).

THEREFORE:

- ✓ **If PARENT compound has been studied in 4 soils, use of geometric mean of DT50s**
- ✓ **If METABOLITES were studied in min. 3 soils, use of geometric mean of DT50s**
- ✓ **In cases where a large number of additional data points are available (*i.e.* 9 or more) , a median values may be more appropriate**
- ✓ **if LESS than the recommended number of soils were studied, use of worst-case results**

Parameters selection for PECgw modelling

Management related to substance/crop parameters (Refer to GAP)

Number of applications: worst case options should be used.

Application rates: worst case options should be used. For all models, the dose should be corrected for the amount of crop interception occurring.

Application dates: worst case options should be used, but realistic values may be used for additional simulations.

Incorporation depth: the majority of applications are likely to be to foliage or to soil surface, and the depth is therefore unnecessary. However, some compounds may be incorporated and in such cases the label recommendation for incorporation depth (usually ca. 20 cm) should be used as input.

Parameters selection for PECgw modelling

MANAGEMENT RELATED TO SUBSTANCE/CROP PARAMETERS (REFER TO GAP)

CROP INTERCEPTION - 1

The actual amount of active substance reaching soil is derived from the maximum application rate reduced by crop interception if plants are present at the time of application. When application is made to bare soil according to the GAP, crop interception is not required.

In other cases, the following tables need to be followed, also checking the bbch monograph

EFSA guidance

Table 1.4: Interception (%) by apples, bushberries, citrus and vines dependent on growth stage

Crop	Stage				
	BBCH# 0–9	BBCH# 10–69		BBCH# 71–75	BBCH# 76–89
Apples	without leaves 50	flowering 60		early fruit development 65	full canopy 65
	BBCH# 0–9	BBCH# 10–69			BBCH# 71–89
Bushberries	without leaves 40	flowering 60		flowering 60	full foliage 75
Citrus	all stages 80				
	BBCH# 0–9	BBCH# 11–13	BBCH# 14–19	BBCH# 53–69	BBCH# 71–89
Vines	without leaves 40	first leaves 50	leaf development 60	flowering 60	ripening 75

#The BBCH code is indicative (Meier, 2001).

Parameters selection for PECgw modelling

Management related to substance/crop parameters (Refer to GAP)

Crop interception - 2

Table 1.5: Interception by other crops dependent on growth stage

Crop	Bare – emergence	Leaf development	Stem elongation		Flowering		Senescence Ripening
	BBCH#						
	0– 09	10–19	20–39		40–89		90–99
Beans (field + vegetable)	0	25	40		70		80
Cabbage	0	25	40		70		90
Carrots	0	25	60		80		80
Cotton	0	30	60		75		90
Grass##	0	40	60		90		90
Linseed	0	30	60		70		90
Maize	0	25	50		75		90
Oil seed rape (summer)	0	40	80		80		90
Oil seed rape (winter)	0	40	80		80		90
Onions	0	10	25		40		60
Peas	0	35	55		85		85
Potatoes	0	15	60		85		50
Soybean	0	35	55		85		65
Spring cereals	0	0	BBCH 20–29*	BBCH 30–39*	BBCH 40–69	BBCH 70–89	80–
			20	80	90	80	
Strawberries	0	30	50		60		60
Sugar beets	0	20	70 (rosette)		90		90
Sunflower	0	20	50		75		90
Tobacco	0	50	70		90		90
Tomatoes	0	50	70		80		50
Winter cereals	0	0	BBCH 20–29*	BBCH 30–39*	BBCH 40–69	BBCH 70–89	80
			20	80	90	80	

#The BBCH code is indicative (Meier, 2001).
##A value of 90 is used for applications to established turf.
*BBCH code of 20–29 for tillering and 30–39 for elongation.

Case study – PELMO vers. 5.5.3

10) Leave default value for plant uptake factor, unless user can adjusted it to measured values, if substance specific uptake factors have been determined in appropriate experiments;

11) Insert henry constant, Koc value, Freundlich exponent

12) Click on *Done*

13) Now we need to calculate the transformation rates for each metabolite given (here only 1) and for CO_2 production (both for parent compound and for each metabolite considered), using the following expression:

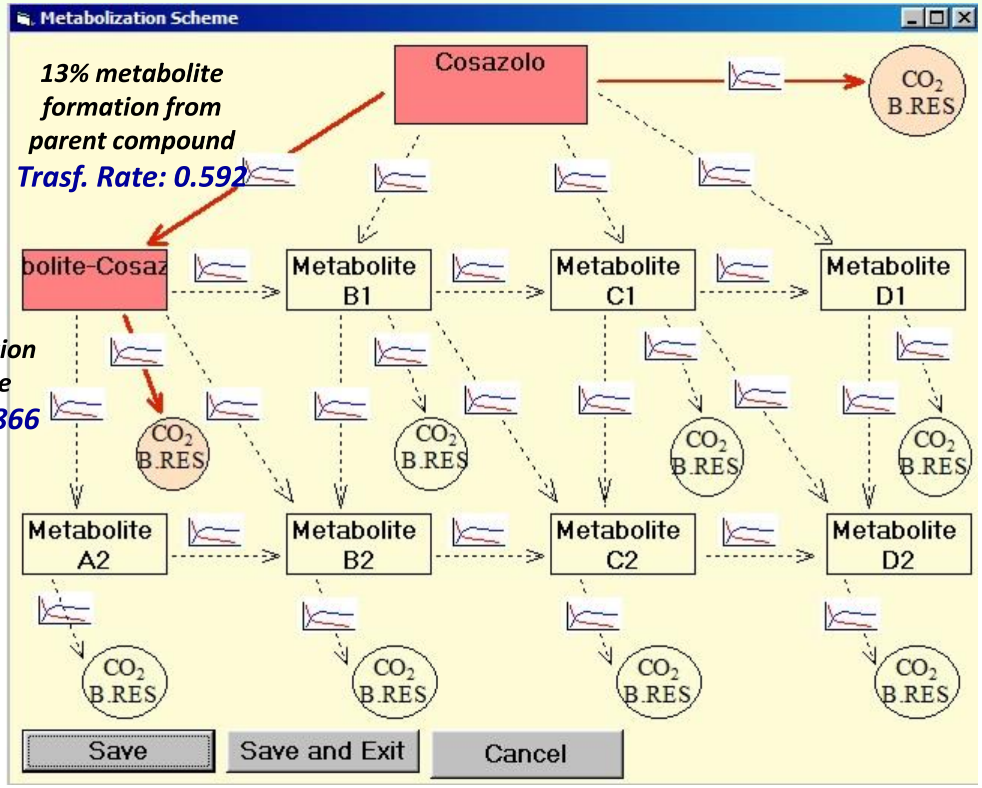
$$\frac{\ln 2}{DT50_{parent} \times (\%metabolite\ or\ CO2/100)}$$

Case study – PELMO vers. 5.5.3

13% metabolite formation from parent compound
Trasf. Rate: 0.592

87% CO2 formation from parent compound
Trasf. Rate: 0.0885

100% CO2 formation from metabolite
Trasf. Rate: 0.0866



Case study – PELMO vers. 5.5.3

14) Save and exit

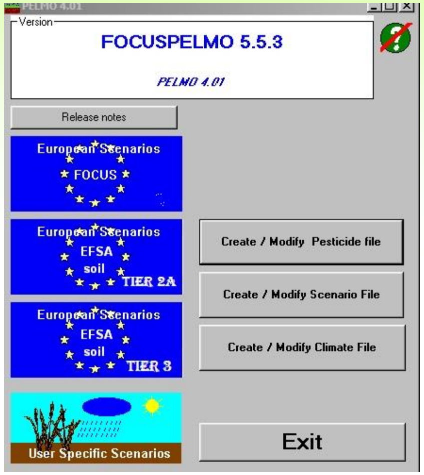
15) Enter on European scenarios FOCUS

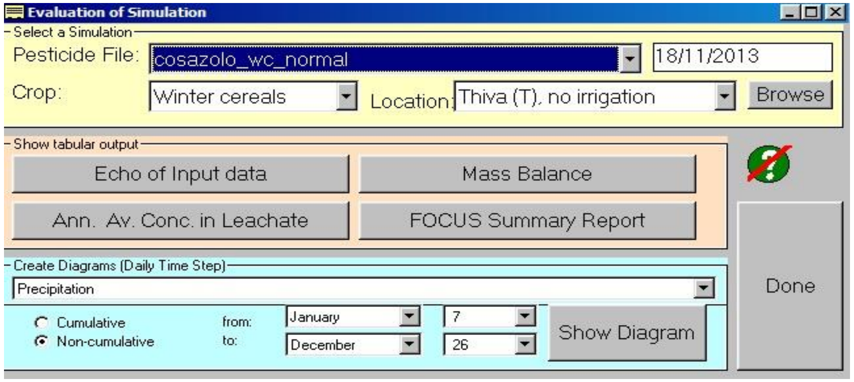
16) Select the crop, select your pesticide file, mark all locations interested for batch

17) Start Batch

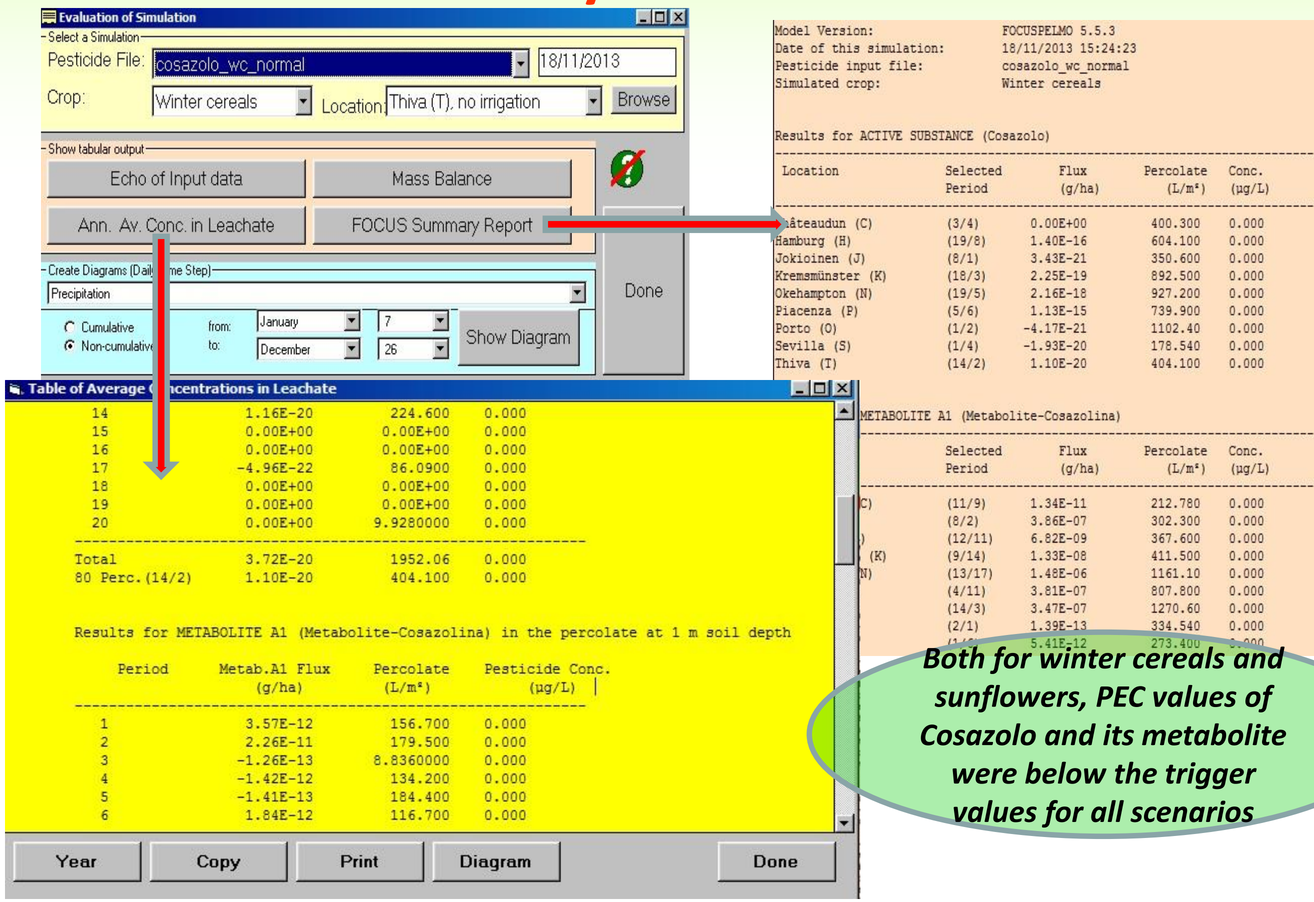
18) Evaluation

17) Input values and output reports are now available



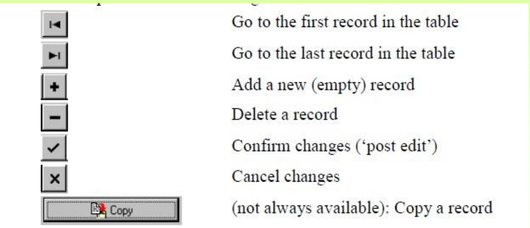


Case study – PELMO vers. 5.5.3



Both for winter cereals and sunflowers, PEC values of Cosazolo and its metabolite were below the trigger values for all scenarios

Case study - PEARL 4.4.4



1) **Edit → substance → click on "+", as insert record**
2) **Input all values reported below inside each record-sheet, and leave default values for other parameters. In Freundlich sorption, for our example case, use "Kom, pH-independent".**

click on optimum moisture

Cosazolo		
Parameter	***Value***	***Unit***
Physical-Chemical features		
Molar mass	153	g/mol
Water Solubility	256	mg/L
Henry constant	3.00E-02	Pa m^3/mol
Saturated vapour pressure	9.50E-06	Pa
Koc	347	mL/g
Freundlich exponent	0.897	Adim.
DT_{50} soil	9	Days
Application features		
Application per year	3	#
Time between application	12	Days
Application rate	0.8	kg/ha
Crops	Winter cereals/Sunflower	
BBCH	12-16/22-25	

Metabolite		
Parameter	***Value***	***Unit***
Physical-Chemical features		
Molar mass	112	g/mol
Water Solubility	347	mg/L
Saturated vapour pressure	6.70E-05	Pa
Koc	476	mL/g
Freundlich exponent	0.987	Adim.
DT50soil	8	Days
DT50wat	0.5	Days
DT50sed	2	Days
Formation from parent in s	13	%

Case study - PEARL 4.4.4

6) Click again on the row created before for the parent compound, and press on “Transformation Scheme” in order to open the relative window

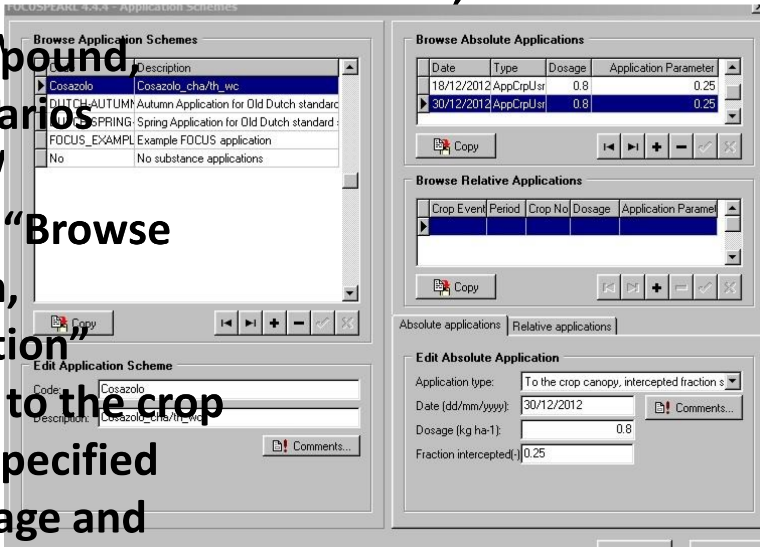
7) Now click on “+”, and select your metabolite from the dropdown list of “Edit metabolite”.

8) Then, insert the metabolite’s fraction transformed, save and close the substance window

9) Edit → we are going to in the “application scheme” w

10) Insert name of parent compound, fill the description of the scenarios in use, and save.

11) Then, edit a new record in “Browse Absolute Applications” section, and fill “Edit Absolute Application” with type of appl. (in this case to the crop canopy, interception fraction specified by the user), date of appl, dosage and fraction intercepted.



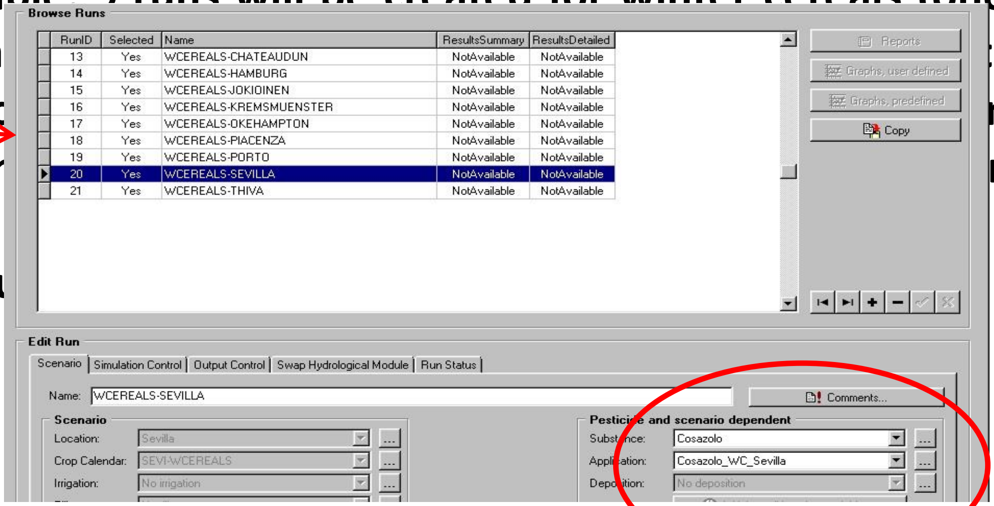
Case study - PEARL 4.4.4

12) Then, click on "Focus wizard", select the crop in use, and all its available scenarios

13) Select your substance and one application scheme from the dropdown list, give a name to your project, and press "Finish"

14) Example: 9 runs will be created for winter cereals (one per scena… …e its applic… …nario deper… …re, a batch…

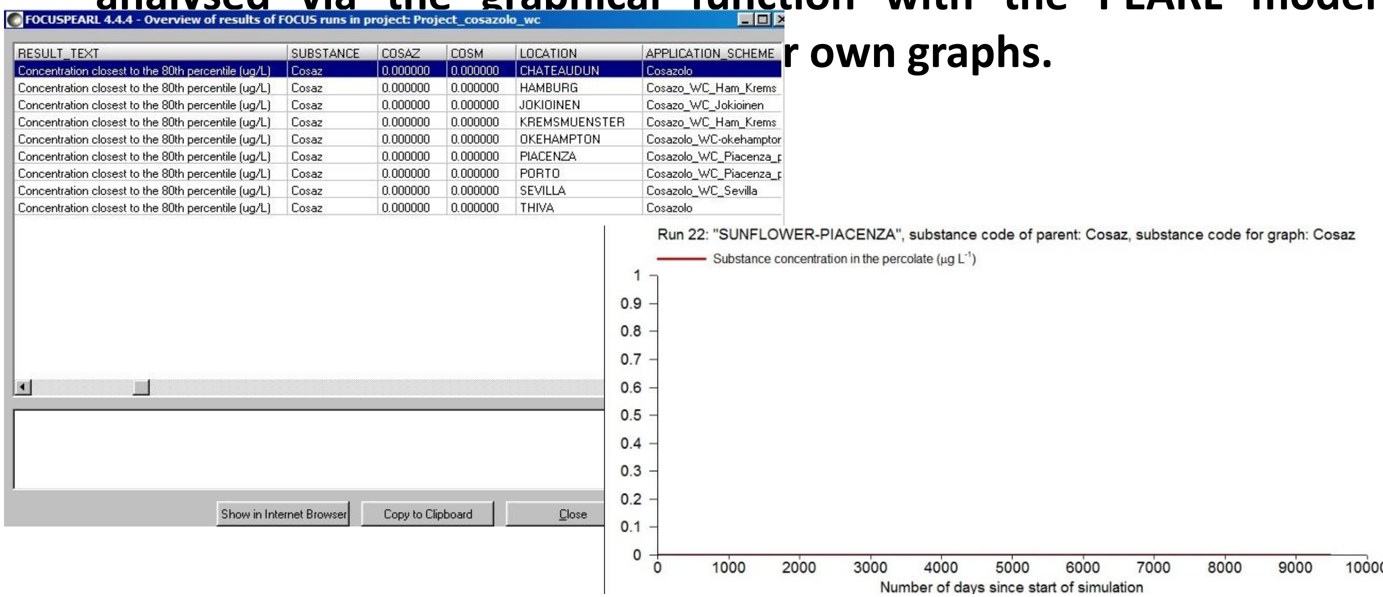
15) Execu…



Case study - PEARL 4.4.4

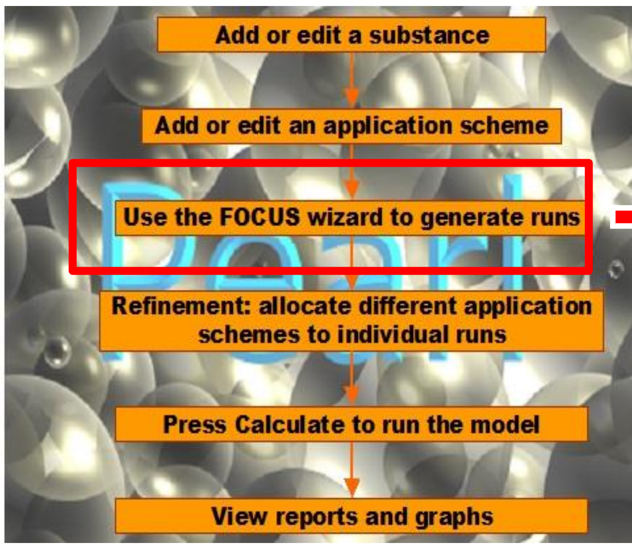
16) Click on “Report” for obtaining the results’ overview, both for parent compound and metabolite.

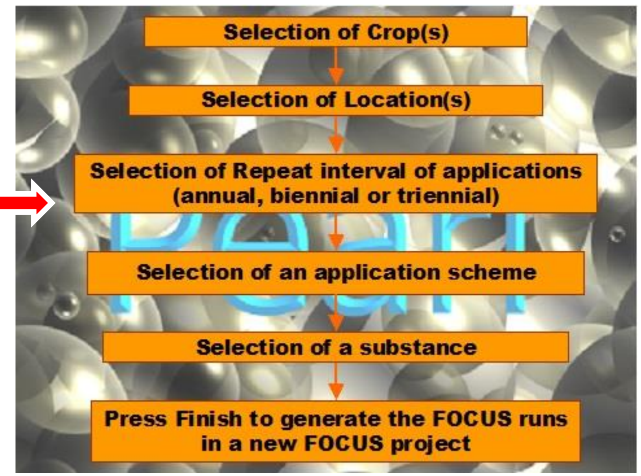
17) After a model run has been completed, the output can be analysed via the graphical function with the PEARL model ... r own graphs.



RESULT_TEXT	SUBSTANCE	COSAZ	COSM	LOCATION	APPLICATION_SCHEME
Concentration closest to the 80th percentile (ug/L)	Cosaz	0.000000	0.000000	CHATEAUDUN	Cosazolo
Concentration closest to the 80th percentile (ug/L)	Cosaz	0.000000	0.000000	HAMBURG	Cosazo_WC_Ham_Krems
Concentration closest to the 80th percentile (ug/L)	Cosaz	0.000000	0.000000	JOKIOINEN	Cosazo_WC_Jokioinen
Concentration closest to the 80th percentile (ug/L)	Cosaz	0.000000	0.000000	KREMSMUENSTER	Cosazo_WC_Ham_Krems
Concentration closest to the 80th percentile (ug/L)	Cosaz	0.000000	0.000000	OKEHAMPTON	Cosazolo_WC-okehamptor
Concentration closest to the 80th percentile (ug/L)	Cosaz	0.000000	0.000000	PIACENZA	Cosazolo_WC_Piacenza_p
Concentration closest to the 80th percentile (ug/L)	Cosaz	0.000000	0.000000	PORTO	Cosazolo_WC_Piacenza_p
Concentration closest to the 80th percentile (ug/L)	Cosaz	0.000000	0.000000	SEVILLA	Cosazolo_WC_Sevilla
Concentration closest to the 80th percentile (ug/L)	Cosaz	0.000000	0.000000	THIVA	Cosazolo

To sum up - PEARL 4.4.4





PEC surface water calculation

EXPOSURE: SURFACE WATER

Major routes of exposure:

SPRAY DRIFT: water much far away from the application area

DRAINAGE: removal of surplus water from land, via within-field drains

RUNOFF: close to treated area. Dependent on the topography, the soil texture, the amount of rain

SPRAYDRIFT

The amount of spraydrift reaching non-target areas is dependent on:

- Distance from the area of application
- Mode of application (formulation, technical equipment)
- Crop (height, growth stage)
- Weather (e.g. wind speed)

Spraydrift deposition generally calculated as:

$DEPOSITION = DOSE_{nominal} \times f_{drift}$

f_{drift} = spraydrift fraction, dependent on crop, growth stage and distance from the target area

RUN-OFF

Occurrence and extent of run-off

- **topography** of the landscape (slope),
- **soil texture** (OC, presence/absence of sand and stone)
- **intensity** of the rain event
- **distance** between the treated area and the receiving ecosystem
- **elapsed time** between pesticide application and onset of rainfall.

Tiered Approach

- STEP 1: Single application, fixed scenario
  STEP 1-2 Calculator
- STEP 2: Multiple applications, regional variation
  STEP 1-2 Calculator
- STEP 3: Advanced modeling, specific European scenarios
  SWASH, PRZM, MACRO, TOXSWA
- STEP 4: Site-specific modeling

FOCUS MODELS

KNOELL ACADEMY

STEP 1/2: Steps 1-2 (**S**urface water **T**ool for **E**xposure **P**redictions – Step 1-2)

Step 1

- Single application of overall application rate, no interception

Step 2

- Single or multiple application, differences in timing of application (Mar-May, Jun-Sep, Oct-Feb), northern or southern europe, interception (depending on crop)

STEP 3: SWASH (**S**urface **WA**ter **S**cenarios **H**elp) mit drei vers. Unterprogrammen

Step 3

- 10 scenarios with realistic combination of climate, crop, soil and agricultural practice
- application method (ground spray, air blast, …)
- applicaton timing based on different crops

STEP 4: SWAN (**S**urface **W**ater **A**ssessment e**N**abler)

Step 4

- reducing of drift entries (buffer strips, drift reducing nozzles)
- reducing of runoff entries (vegetated filter strips)

STEPS 1&2

STEP1

- Not correlated to climate, soil topography, crop.
- Drift values have been calculated at the 90th percentile from BBA (2000). Values for a 1m “no spray zone” for arable crops and a 3m “no spray zone” for vines, orchards and hops have been selected
- At Step 1 the run-off/erosion/drainage loading to the water body was set at 10% of the application for all scenarios.
- At Step 1, degradation in the water and sediment compartments is dependent on the DT50sediment/water (combined water + sediment value).

STEP2

- Refinement
- Degradation is assumed to follow first-order kinetics in soil, surface water and sediment
- Drift loadings: The fraction of each application reaching the adjacent water is both a function of method and number of applications.
- the amount of pesticide that enters the soil at Step 2 is corrected for crop interception.
- Four days after the final application, a run-off/erosion/drainage loading is added to the water body. This loading is a function of the residue remaining in soil after all of the treatments (g/ha) and the region and season of application.
- In common with Step 1, the run-off/erosion/drainage entry is distributed between water and sediment at the time of loading according to the Koc of the compound.

PEC surface water calculation

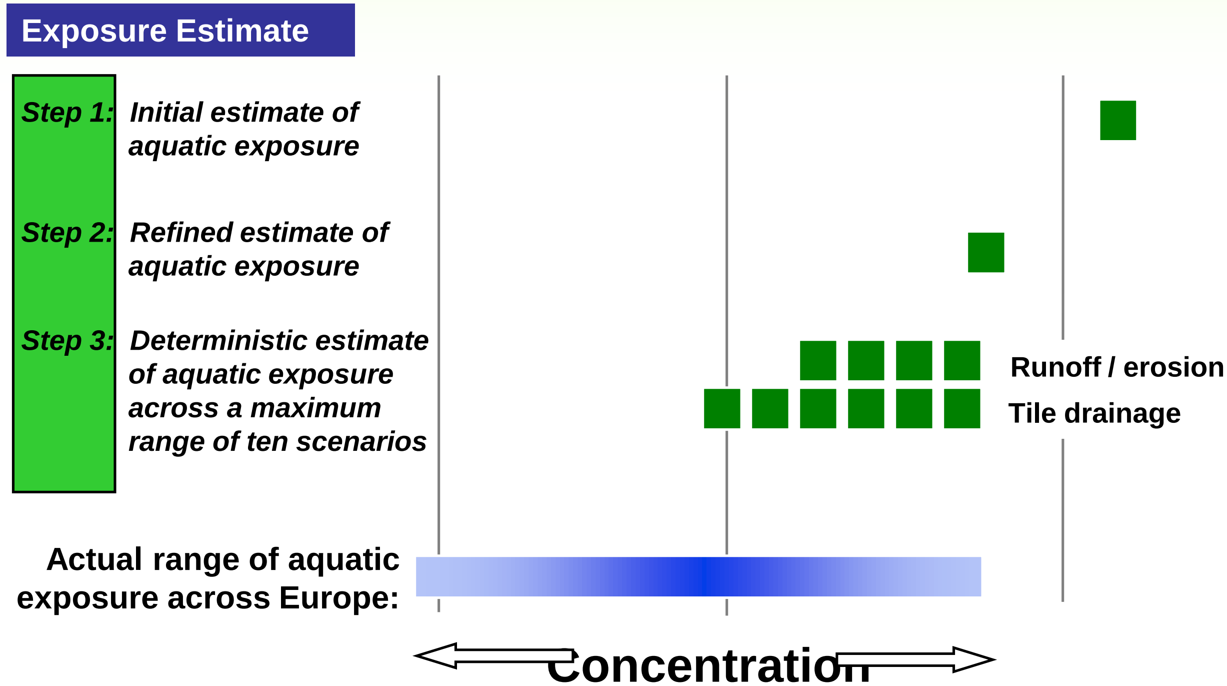
STEP 1 input data

- solubility
- adsorption coefficient Koc
- molecular weight a.i. and metabolite
- met maximum % in w/s studies
- met maximum % in soil studies
- degradation rate in water/sediment **(no DT_{50} in water!!!)**

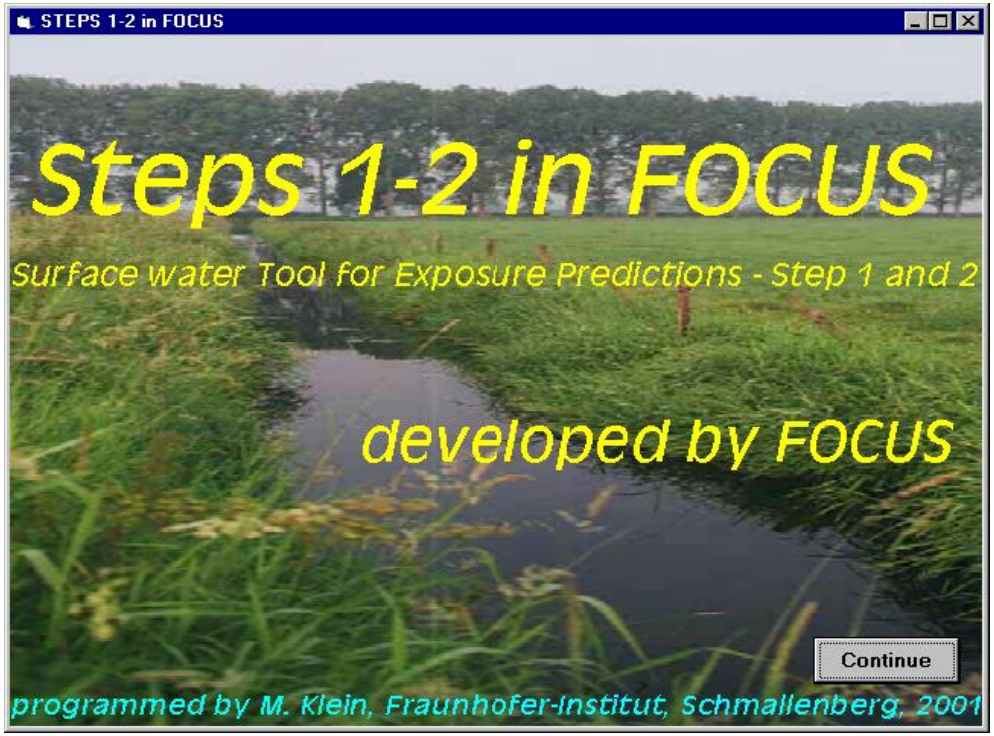
STEP 2 input data

- Same set of data of step 1, than:
- degradation rate in water phase
- degradation rate in sediments
- degradation rate in soil
- number of applications, crop type, amount intercepted, area of use in EU

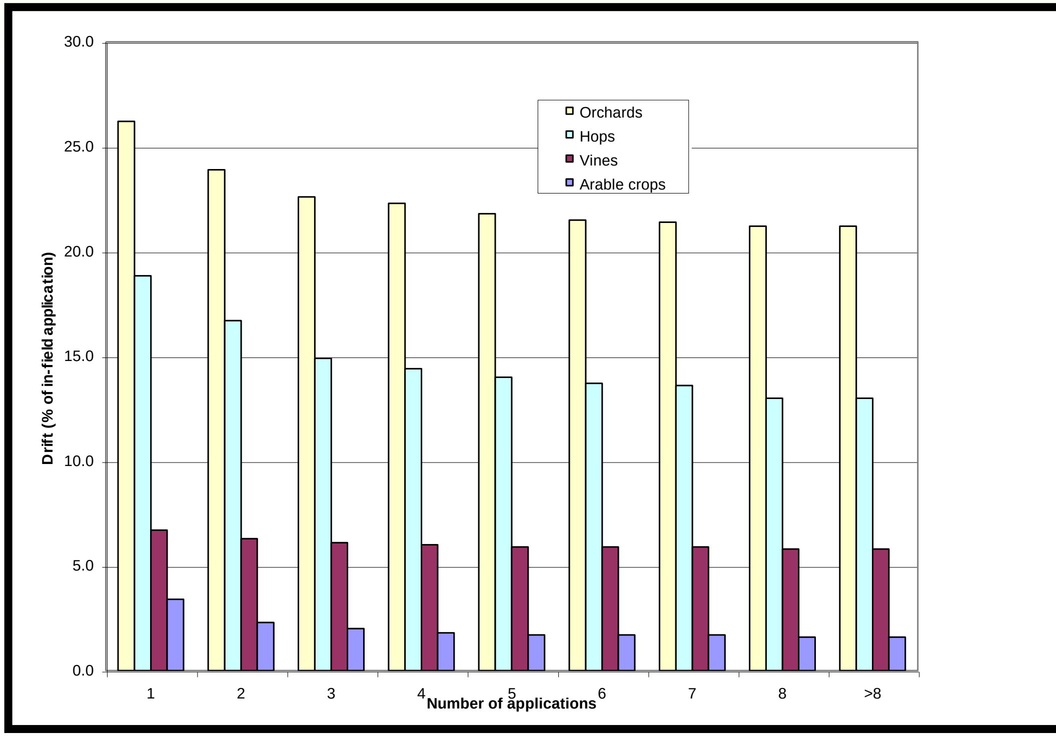
Logic of the FOCUS Approach



Step 1 and 2 model

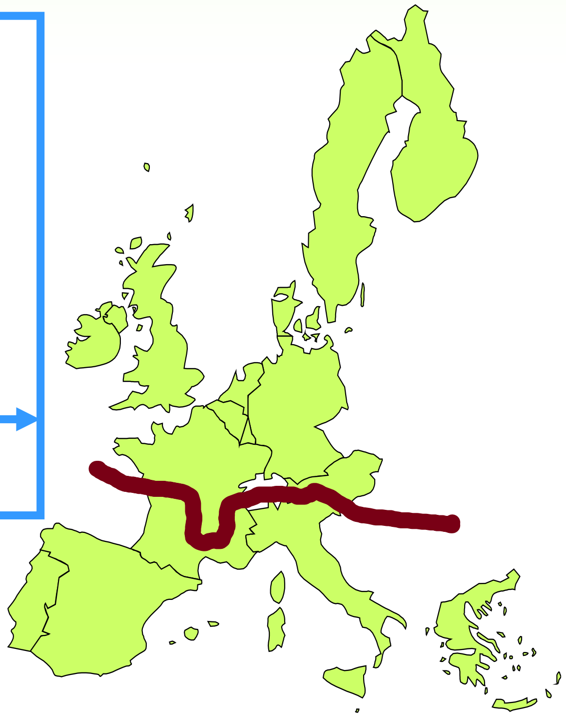


Step 1 and 2: Drift Loadings

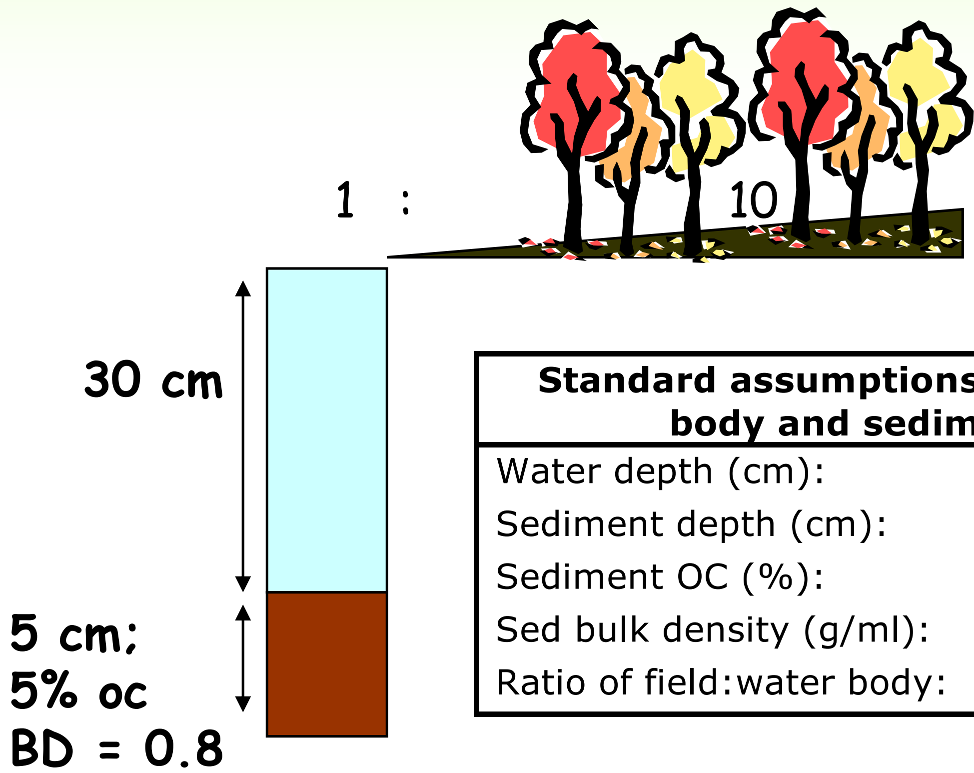


Step 1 and 2: Runoff and Drainage Assumptions

Application Step/Location	Aut	Percent of Spr	Sum
1 / all	10	10	10
2 / North	2	5	2
2 / South	3	4	4



Step 1 and 2: Scenario Assumptions



Standard assumptions for water body and sediment	
Water depth (cm):	30
Sediment depth (cm):	5
Sediment OC (%):	5
Sed bulk density (g/ml):	0.8
Ratio of field:water body:	10

Step 1 and 2: Chemical Data

Chemical properties

- solubility

- sorption coefficient
- degradation rates in soil, water and sediment

Additional data for metabolites

- MW of parent and metabolite
- maximum observed in soil studies
- maximum observed in water/sediment studies

Application data

- rate per application

- number of applications
- type of crop

- extent of canopy interception
- region of use within EU

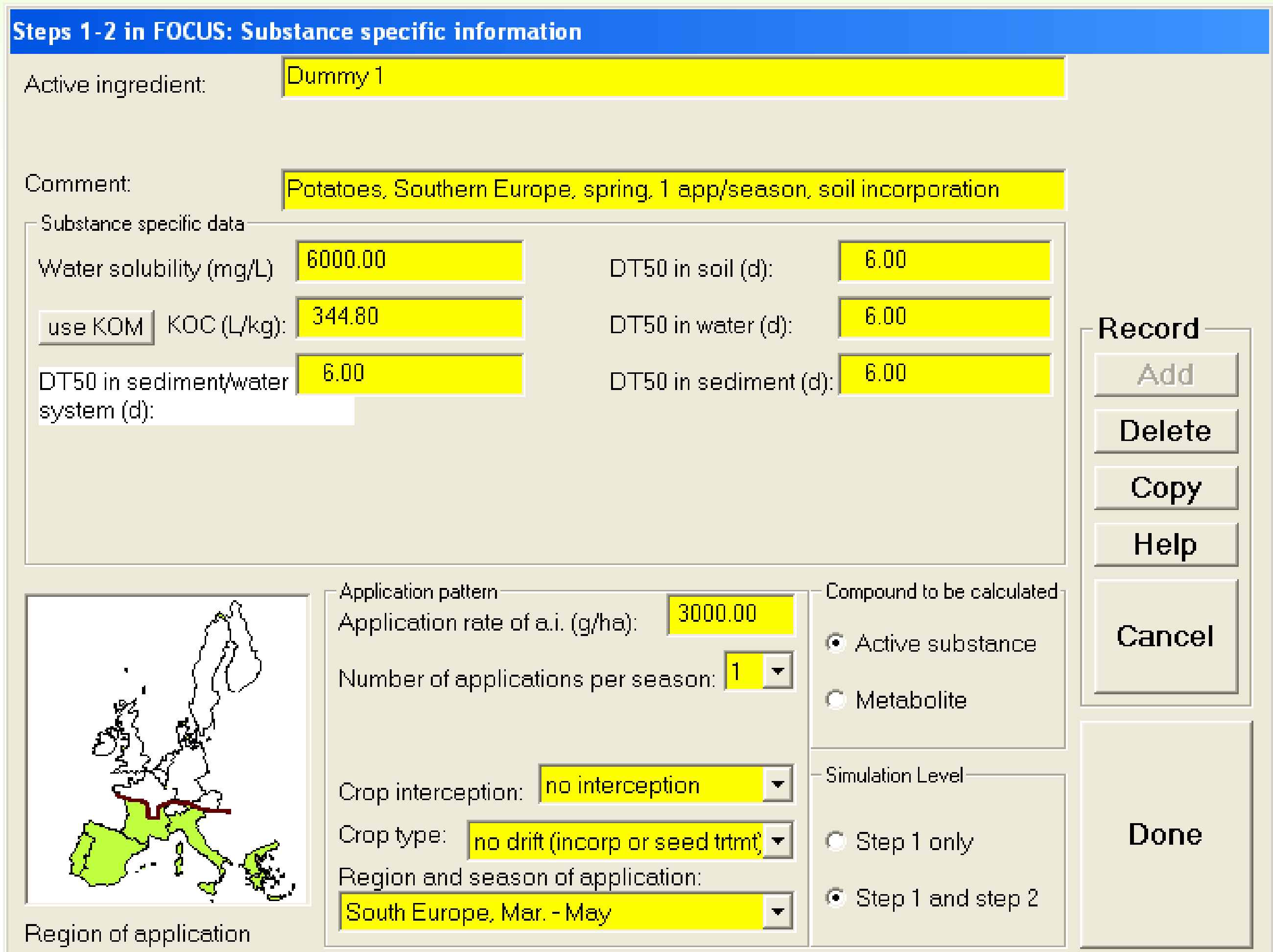
STEP 2: Crop interception

crop	no interception	minimal crop cover	average crop cover	full canopy
cereals, spring	0	0.25	0.5	0.7
cereals, winter	0	0.25	0.5	0.7
citrus	0	0.7	0.7	0.7
cotton	0	0.3	0.6	0.75
field beans	0	0.25	0.4	0.7
grass / alfalfa				0.75
hops				0.7
legumes				0.7
maize				0.75
oil seed rape, spr				0.75
oil seed rape, wir				0.75
olives				0.7
pome / stone frui				0.7
pome / stone frui				0.7
potatoes				0.7
soybeans				0.75
sugar beet				0.75
sunflower	0	0.2	0.5	0.75
tobacco	0	0.2	0.7	0.75
vegetables, bulb	0	0.1	0.25	0.4
vegetables, fruiting	0	0.25	0.5	0.7
vegetables, leafy	0	0.25	0.4	0.7
vegetables, root	0	0.25	0.5	0.7
vines, early applns	0	0.4	0.5	0.7
vines, late applns	0	0.4	0.5	0.7
appln, aerial	0	0.2	0.5	0.7
appln, hand (crop < 50 cm)	0	0.2	0.5	0.7
appln, hand (crop > 50 cm)	0	0.2	0.5	0.7
no drift (incorp/seed trtmt)	0	0	0	0

4 Classes for each crop

- no interception
- minimal crop cover
- average crop cover
- full canopy

PECsw calculation: data input



PECsw calculation: default data

Steps 1-2 in FOCUS: Scenarios for Surface Water

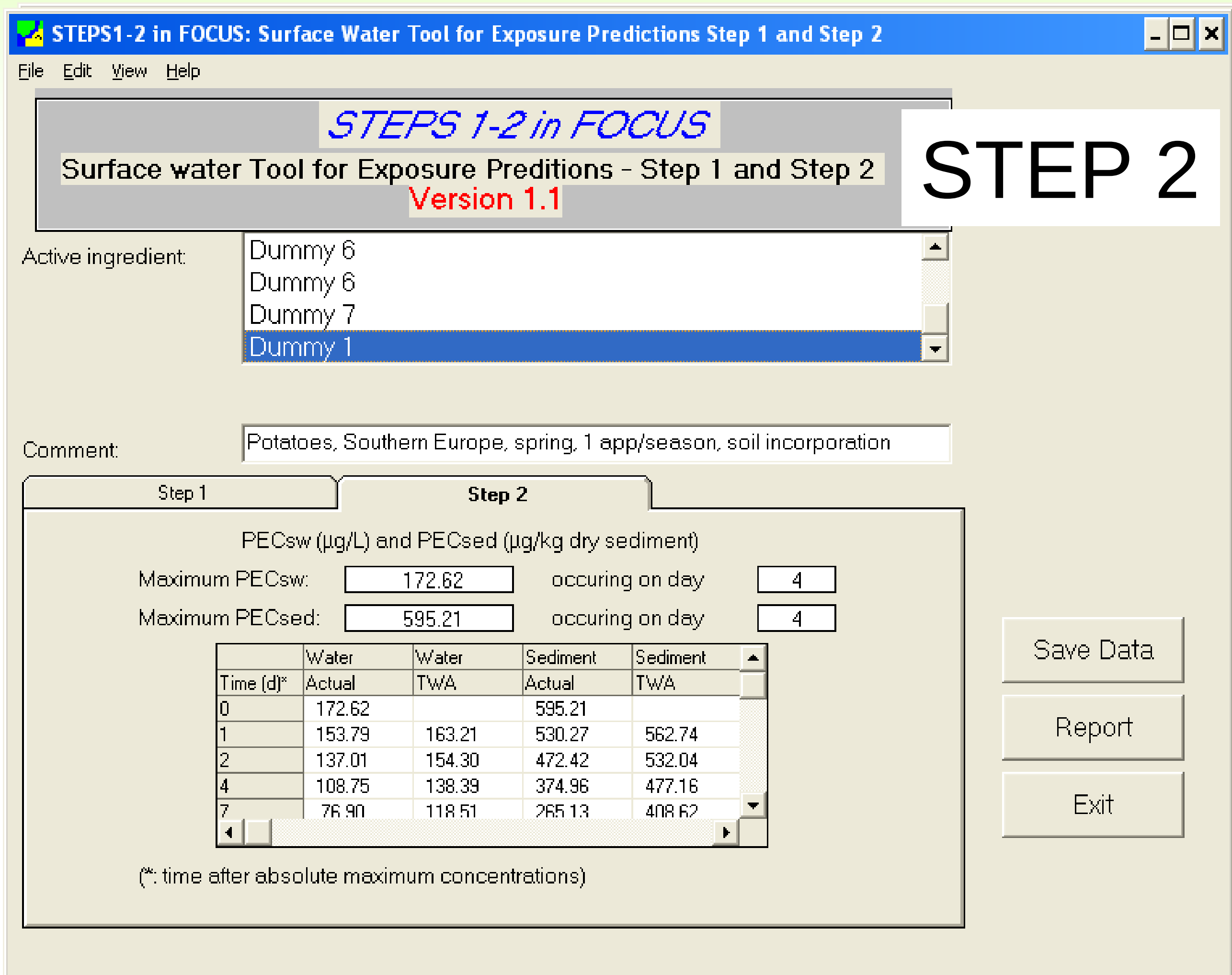
Step 1: Input route assumptions | Step 2: Input route assumptions | Step 2: Crop interception | Surface water definitions

Surface water definitions

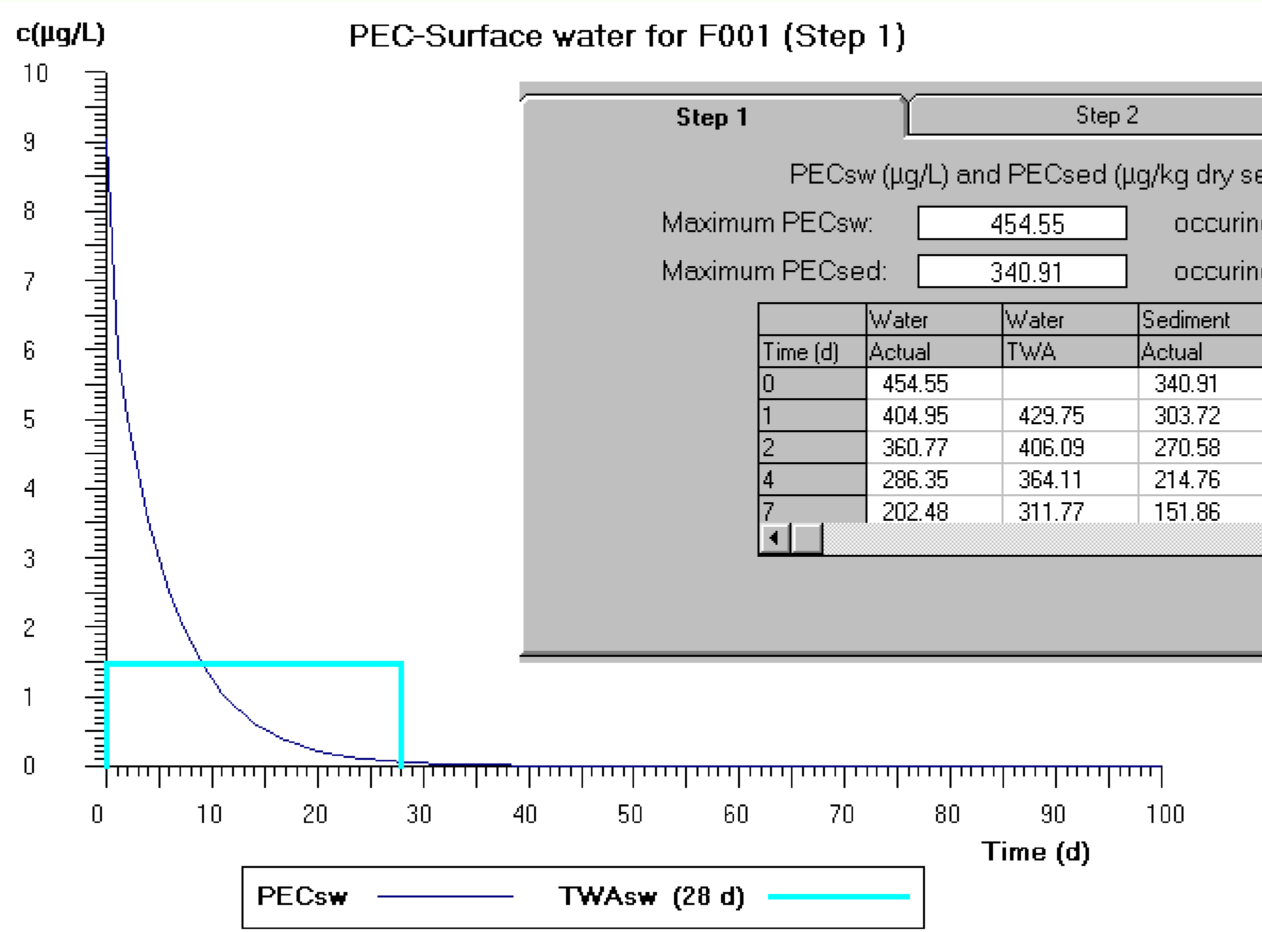
Parameter	Value
Water depth (cm)	30
Sediment depth (cm)	5
Effective sediment depth (cm)	1
Sediment organic Carbon (%)	5
Sediment bulk density (kg/L)	0.8
Ratio of field / water body	10

Copy into Clipboard | Done

PECsw calculation: results



Step 1: Example Results



Step 1 | Step 2

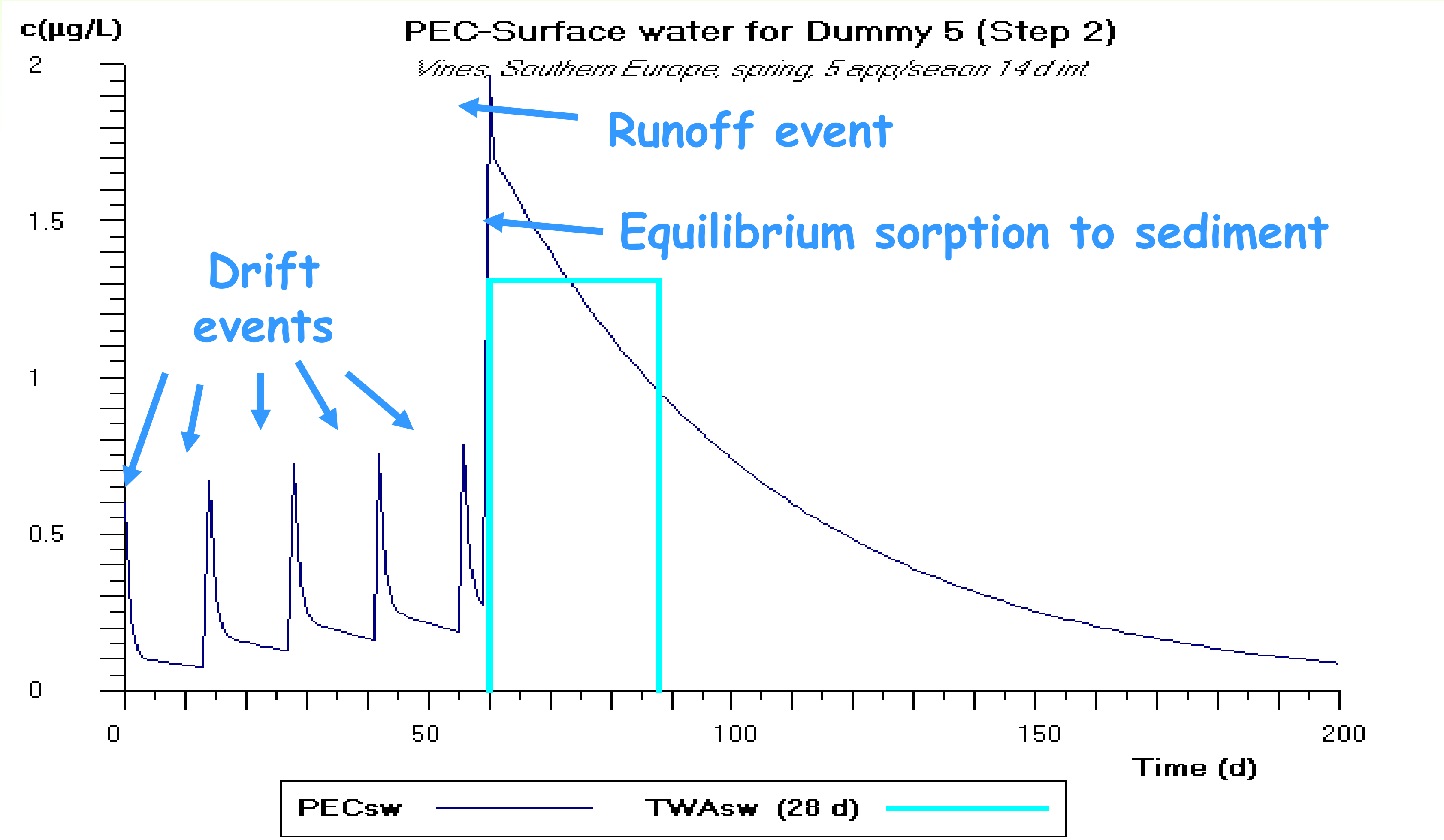
PECsw (µg/L) and PECsed (µg/kg dry sediment)

Maximum PECsw: 454.55 occuring on day 0

Maximum PECsed: 340.91 occuring on day 0

Time (d)	Water Actual	Water TWA	Sediment Actual	Sediment TWA
0	454.55		340.91	
1	404.95	429.75	303.72	322.31
2	360.77	406.09	270.58	304.57
4	286.35	364.11	214.76	273.08
7	202.48	311.77	151.86	233.83

Step 2: Example Results for Water

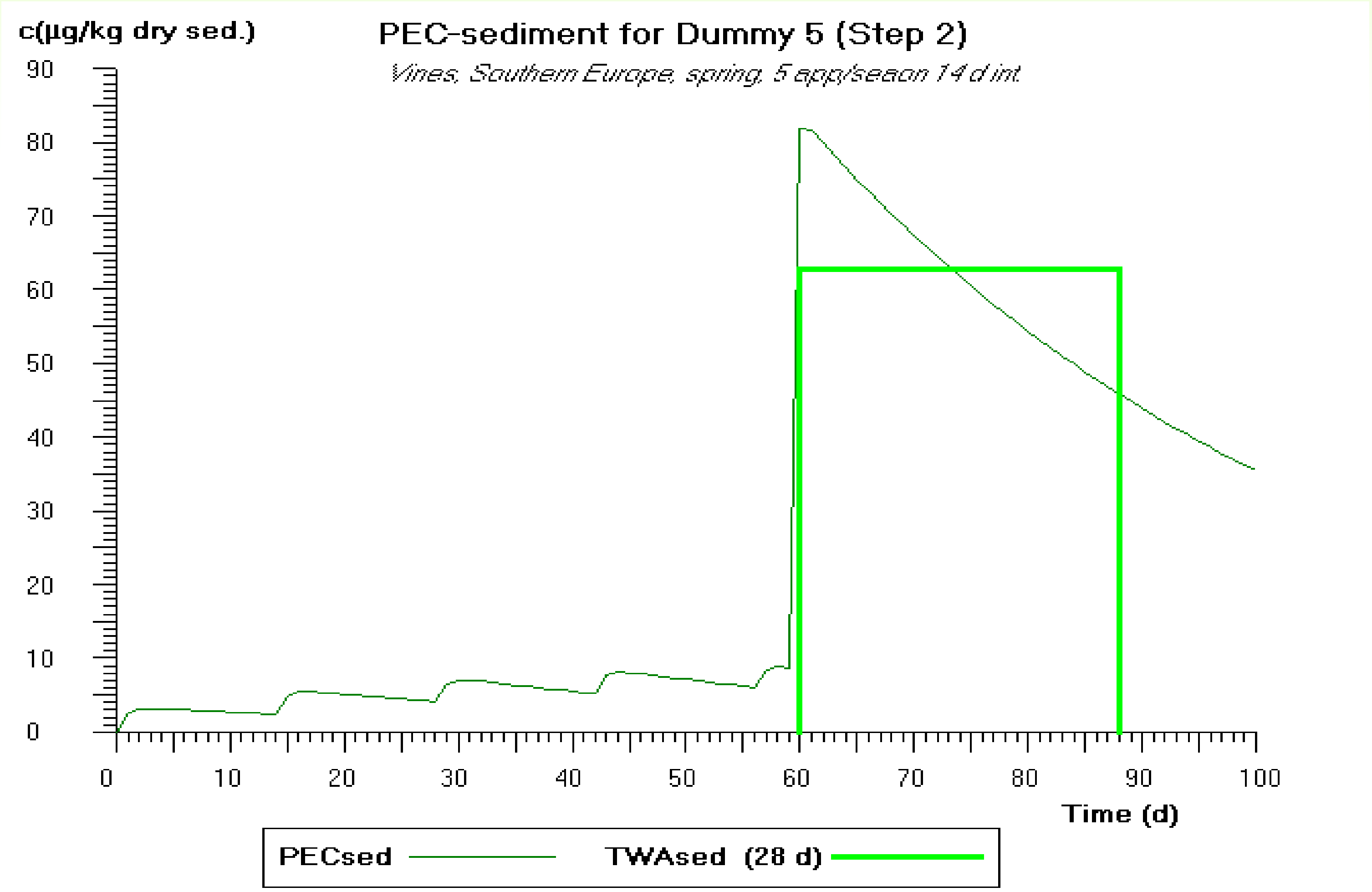


Centro Internazionale per gli Antiparassitari e la Prevenzione Sanitaria

Ospedale Luigi Sacco POLO UNIVERSITARIO

Sistema Socio Sanitario Regione Lombardia ASST Fatebenefratelli Sacco

Step 2: Example Results for Sediment



STEP3 – Swash shell

10 SCENARIOS (6 FOR DRAINAGE, 4 FOR RUN-OFF) identified according to the worst case nature of their inherent agro-environmental characteristics: climate, soil, slope (cropped land does not occur in areas with average slopes > 15%; drainage occurs predominantly on areas with slopes of 4% or less).

- D1 Lanna
- D2 Brimstone
- D3 Vredepeel
- D4 Skousbo
- D5 La Jailliere
- D6 Váyia, Thiva
- R1 Weiherbach
- R2 Valadares, Porto
- R3 Ozzano, Bologna
- R4 Roujan

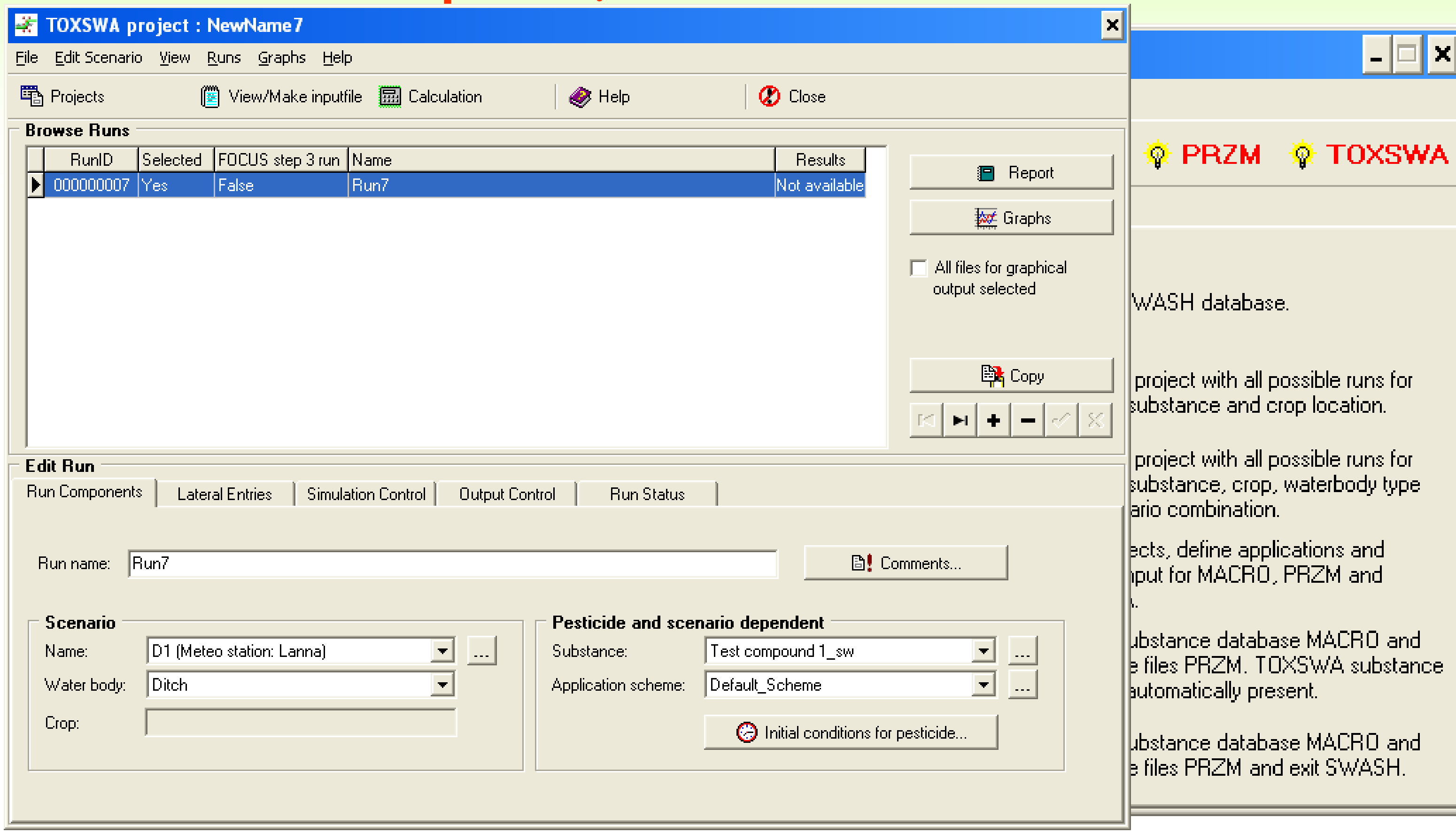
Realistic combination of worst case characteristics for drainage and runoff!

Six of the scenarios characterise inputs from drainage and spray drift whilst four characterise inputs from runoff and spray drift.

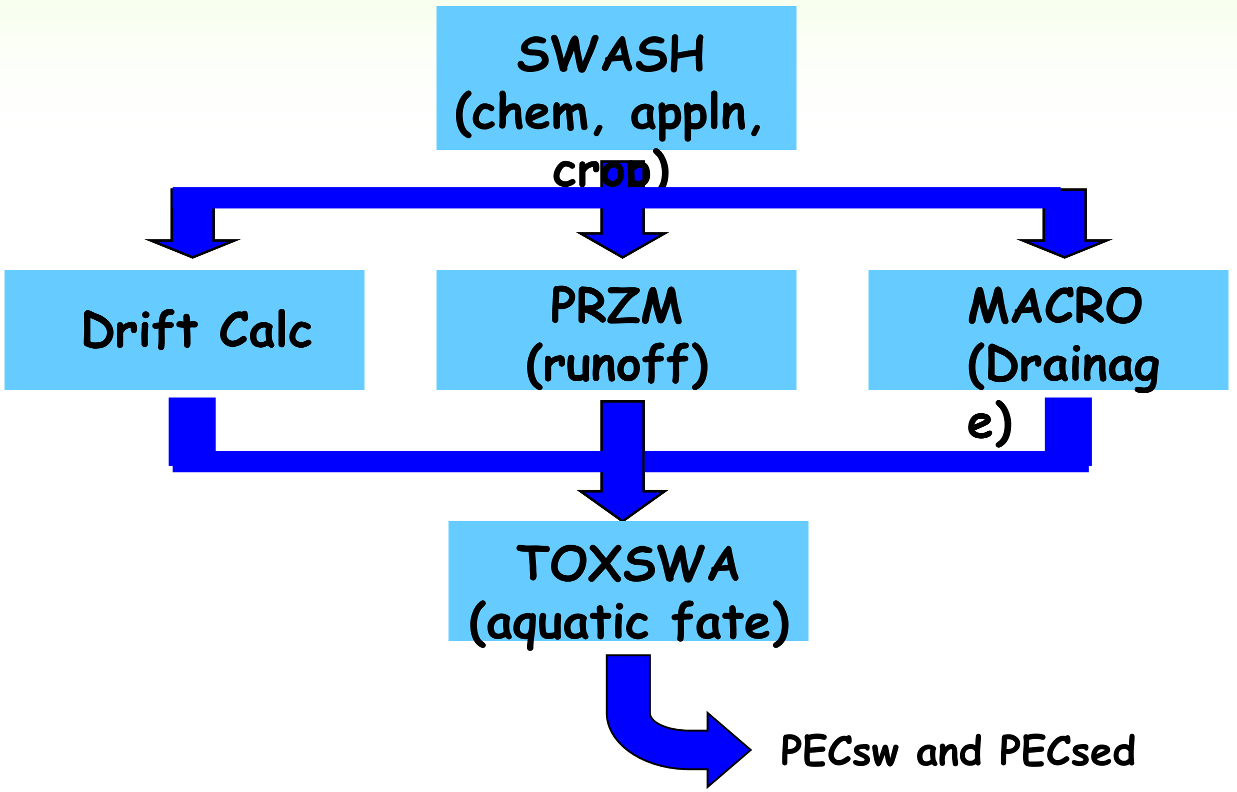
STEP3 – Swash shell

- The model MACRO was chosen to calculate drainage inputs to surface water bodies.
- The Pesticide Root Zone Model (PRZM) was selected to calculate runoff and erosion loadings into surface water bodies for four of the Step 3 FOCUS surface water scenarios.
- The TOXSWA model describes the behaviour of pesticides in a water body at the edge-of-field scale, i.e. a ditch, pond or stream adjacent to a single field. It calculates pesticide concentrations in the both the water and sediment layers.
- TOXSWA considers four processes: (i) Transport, (ii) Transformation, (iii) Sorption and (iv) Volatilisation. The TOXSWA model does not simulate the drainage or runoff/erosion processes itself, but uses the fluxes calculated by other models as entries into the water body system of TOXSWA.
- TOXSWA in FOCUS does not simulate the formation of metabolites in water or in sediment.

Step 3 models



STEP 3 CALCULATIONS



USER-DEFINED INPUTS (entered in SWASH)

- Chemical data

  parent / daughter relationships

  chemical properties of parent/ daughter

- Application data

  rate per application

  number of applications

  application window (earliest and latest dates)

- Crops and scenarios

  crop type (23 different crops)

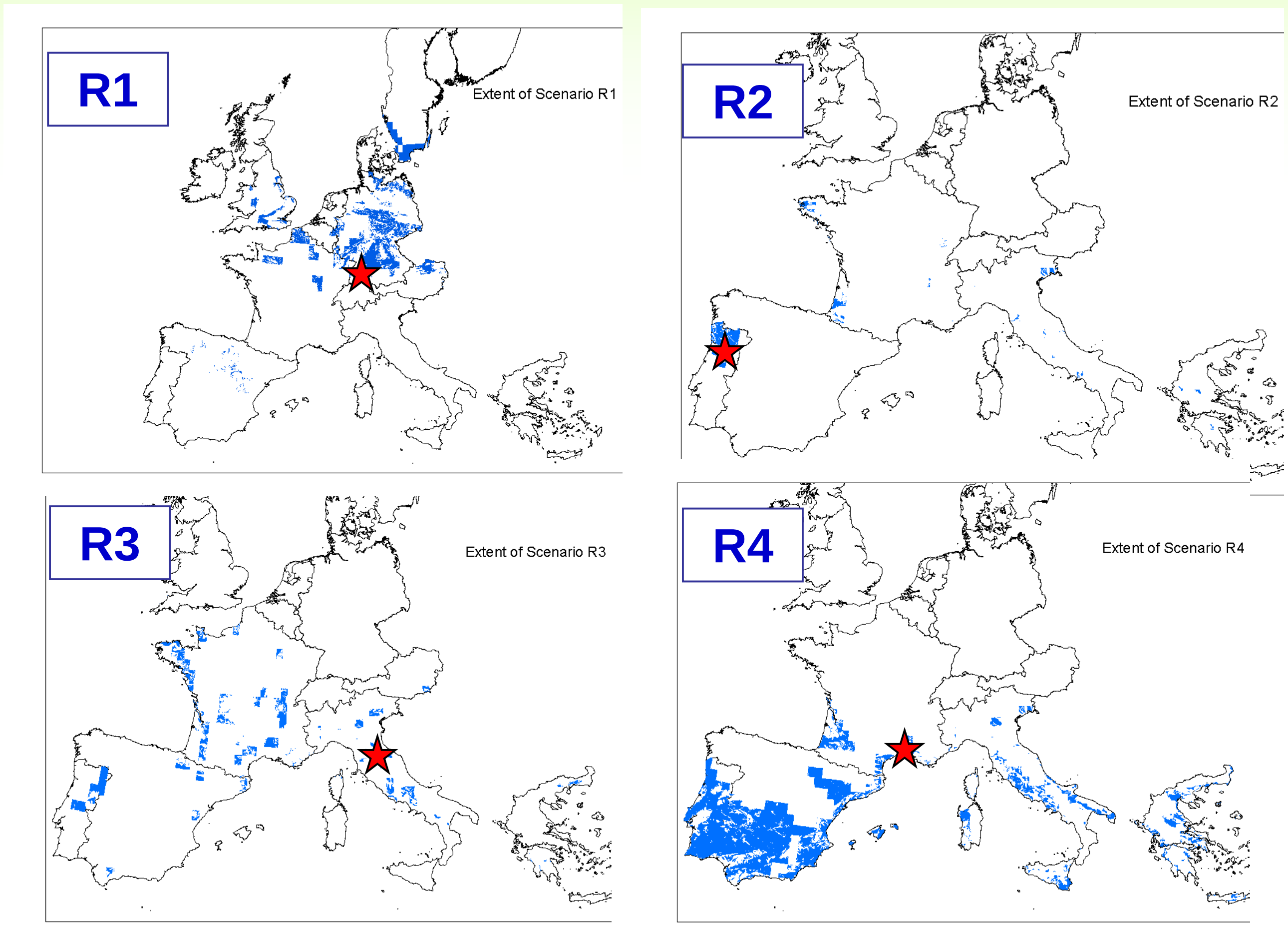
  scenarios (6 drainage and 4 runoff)

  appropriate scenarios are defined for crop

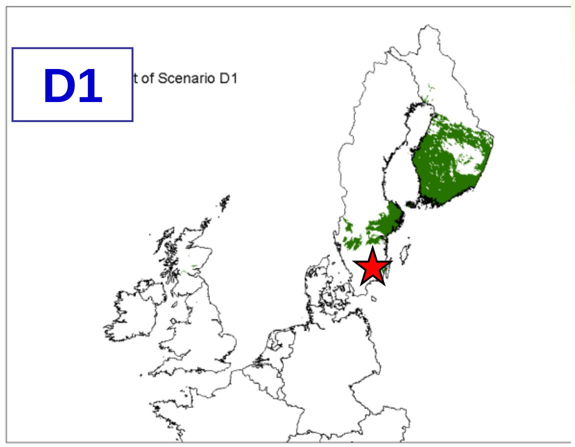
FIXED SCENARIO PARAMETERS

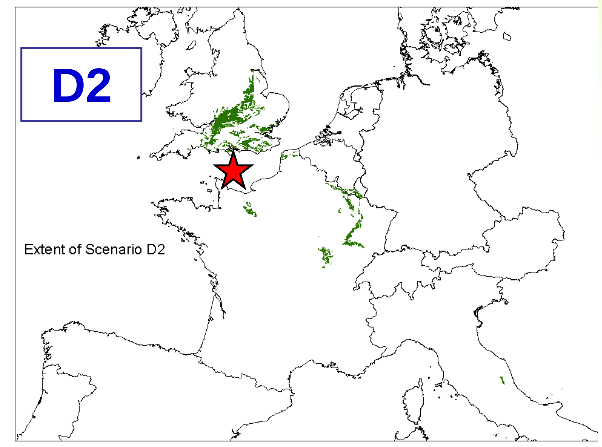
- Agronomic data
  - cropping dates (planting, maturation, harvest) growth data (root depth, plant height, canopy)
- Soil data
  - properties of soil profile
  - topographical data (slope, field dimensions)
- Climatic data (daily)
  - precipitation (and irrigation, if appropriate)
  - evapotranspiration
  - temperature
- Water body types
  - ditch, pond and stream
  - dynamic hydrology with upstream catchments

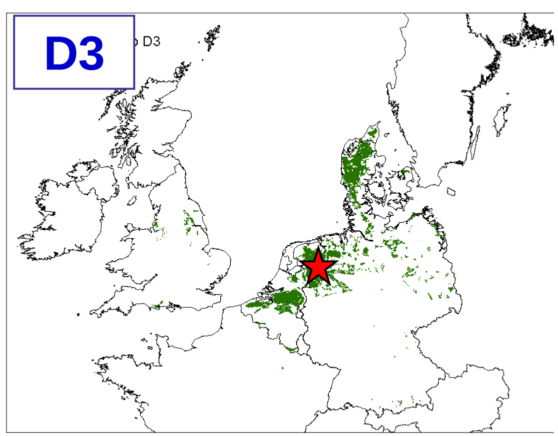
Extent of FOCUS runoff scenarios

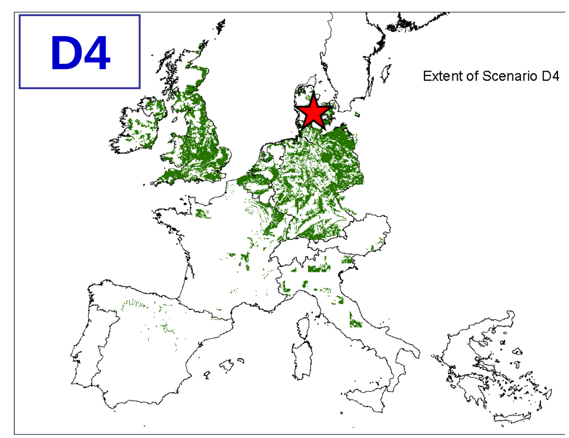


Extent of FOCUS drainage scenarios

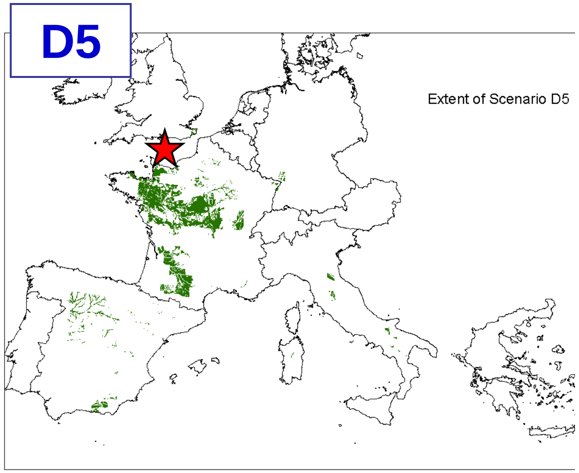


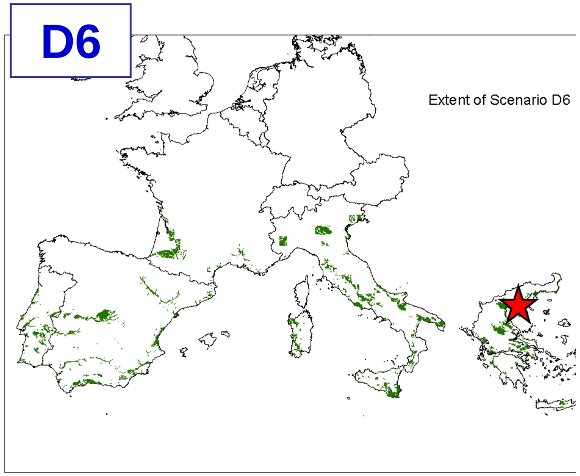






Extent of FOCUS drainage scenarios (continued)





Calculated scenario parameters

- <u>Application dates</u>

  specific application dates are calculated by Pesticide Application Tool (PAT) within PRZM:

- avoids application on days with precipitation
- ensures precipitation within 10 days of appln

- <u>Simulation dates</u>

  depending upon the date of the first application, a specific simulation period is selected for simulation:

  - 12 months for PRZM

  - 16 months for MACRO

Calculations performed by PRZM and MACRO

- PRZM results represent edge-of-field runoff and erosion containing water, soil and chemical; MACRO results represent tile drainage from beneath treated fields

- Most scenarios have available runoff or drainage data from field experiments for comparison
- For selected year, outputs include:
  - hourly runoff or drainage volume
  - hourly chemical concentration
- Output files are transferred to TOXSWA for simulation of aquatic fate

PEC surface water mitigation

STEP 4: generally used to introduce mitigations to be reported in the label according Commission Regulation (EU) No 547/2011of 8 June 2011.

Which water bodies are to be protected?
To be defined before starting with the evaluation.

All surface waters, whether natural or artificial, are to be considered relevant <u>EXCEPT</u>:

- **Overflow ditches: ditches running alongside cultivated fields for the collection of excess water.**
- **Irrigation reservoirs/outlets: Water sources intended only or the irrigation.**
- **•Perched aquifers: Water sources whose water level is at least one meter above the level of the crop treated.**

SW/SED input values

- **DT50 soil**: geometric mean (normalised)
- **Koc**: minimum value, or arithmetic mean
- **DT50 water, sediment, whole system**: generally arithmetic mean, or worst-case.

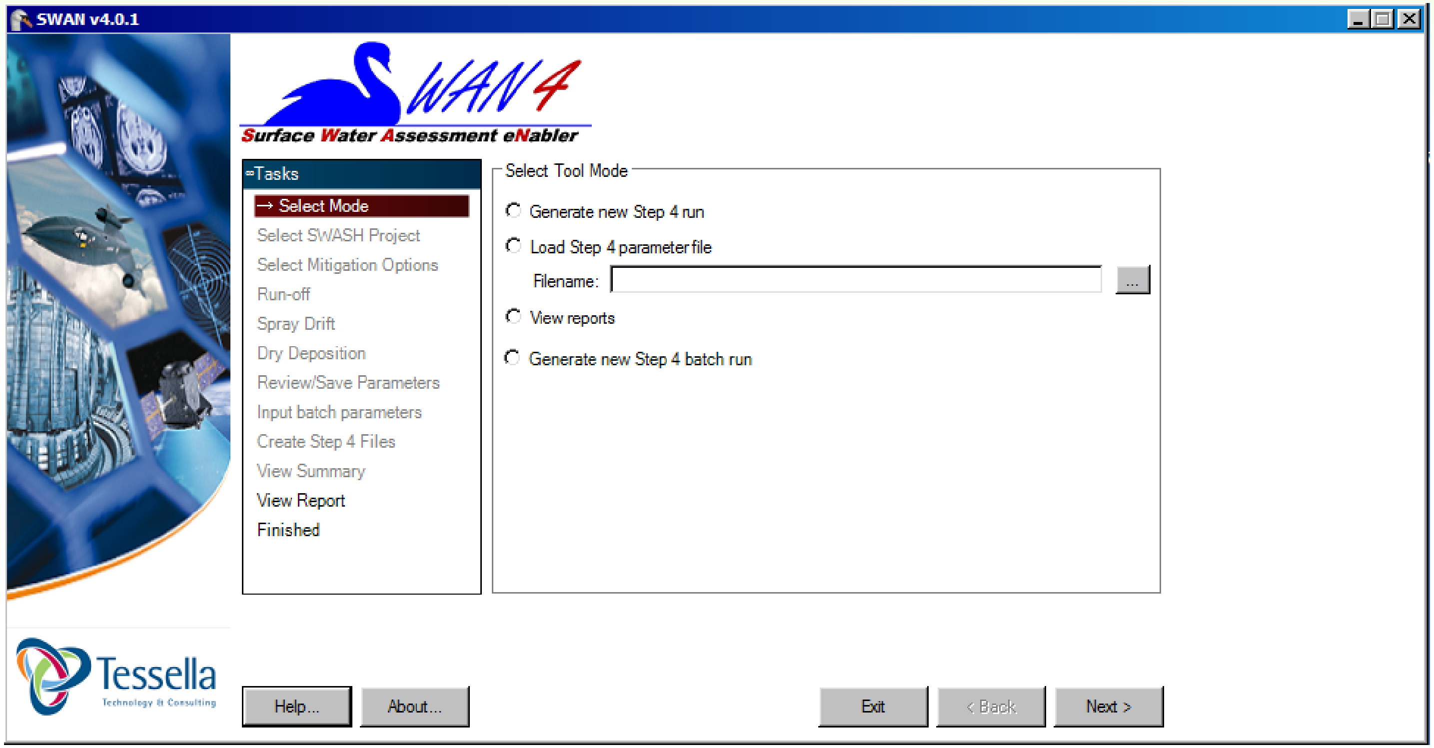
STEP4 - SWAN

- **Mitigation measures are incorporated into Step 3 10 scenarios (resulting in a Step 4 calculation)**

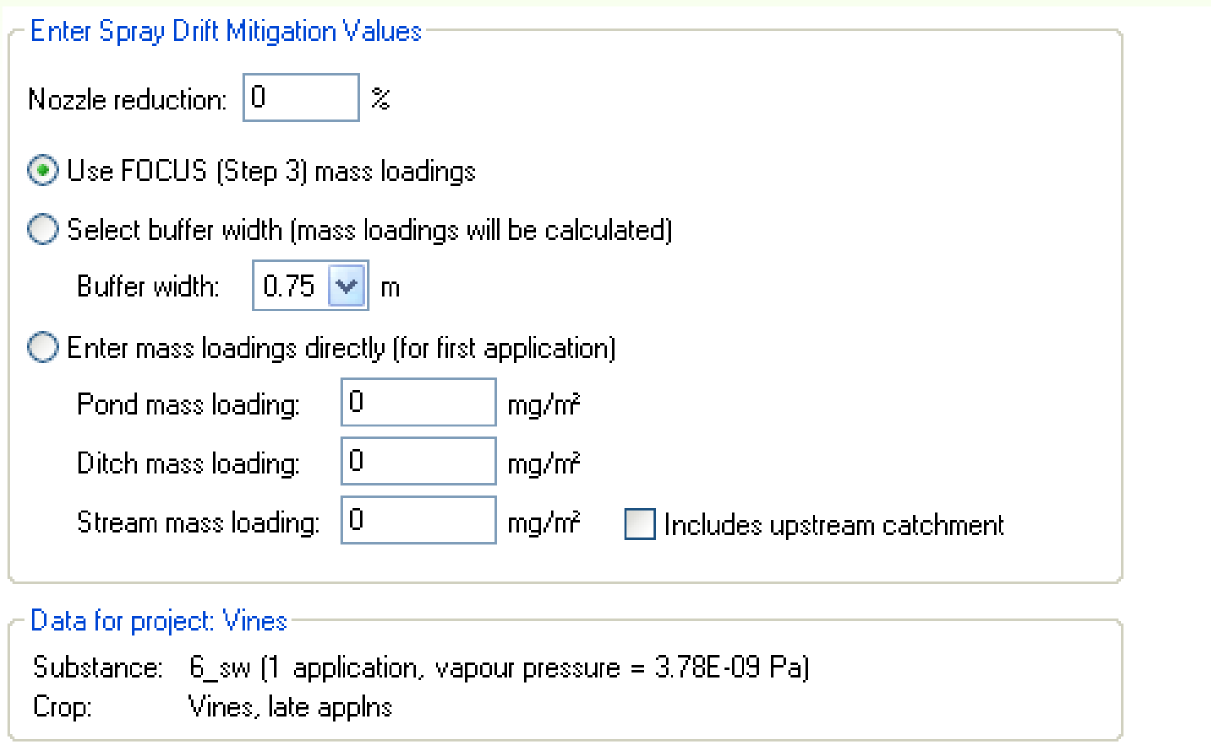
Table 7. 90th percentile worst-case values for reduction efficiencies for different widths of vegetated buffers and different phases of surface runoff

Buffer width (m)	10-12	18-20
Reduction in volume of runoff water (%)	60	80
Reduction in mass of pesticide transported in aqueous phase (%)	60	80
n (for aqueous phase)	*36*	*30*
Reduction in mass of eroded sediment (%)	85	95
Reduction in mass of pesticide transported in sediment phase (%)	85	95
n (for sediment phase)	*19*	*11*

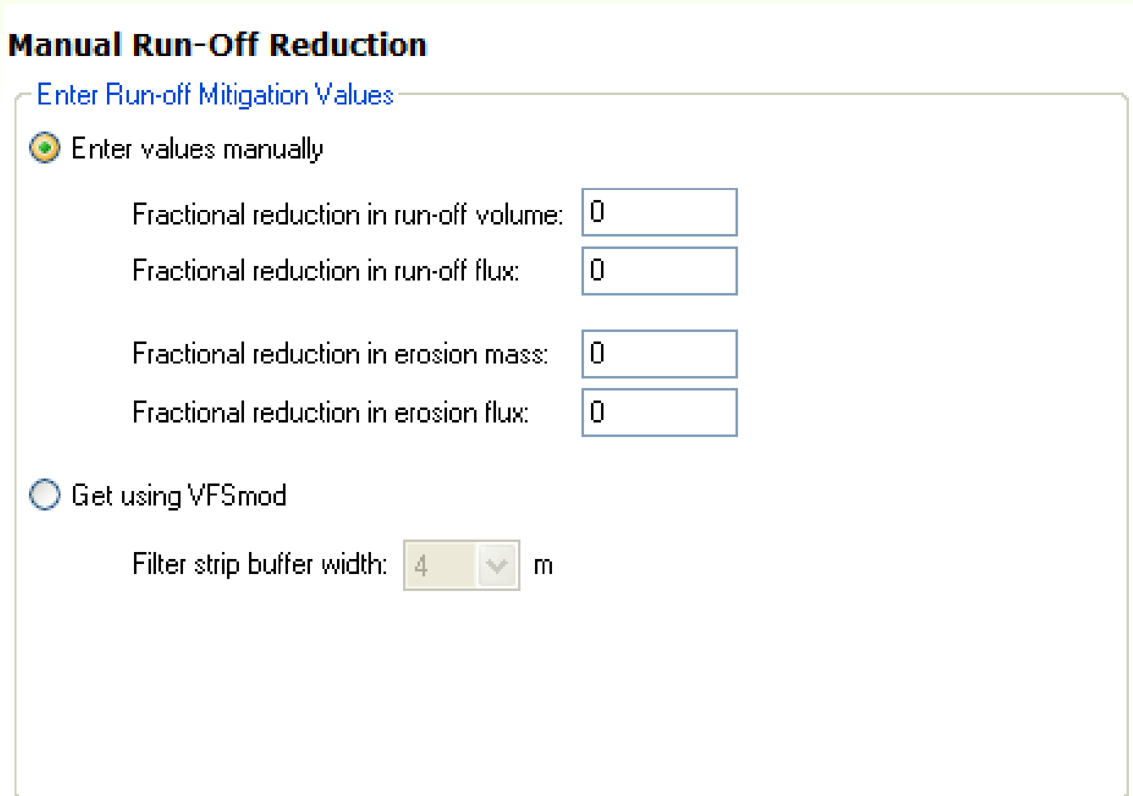
Model


SWAN v4.0.1
SWAN 4
Surface Water Assessment eNabler
Tasks
→ Select Mode
Select SWASH Project
Select Mitigation Options
Run-off
Spray Drift
Dry Deposition
Review/Save Parameters
Input batch parameters
Create Step 4 Files
View Summary
View Report
Finished
Select Tool Mode
Generate new Step 4 run
Load Step 4 parameter file
Filename:
...
View reports
Generate new Step 4 batch run
Tessella
Technology & Consulting
Help...
About...
Exit
< Back
Next >

Model


Enter Spray Drift Mitigation Values
Nozzle reduction: 0 %
Use FOCUS (Step 3) mass loadings
Select buffer width (mass loadings will be calculated)
Buffer width: 0.75 m
Enter mass loadings directly (for first application)
Pond mass loading: 0 mg/m²
Ditch mass loading: 0 mg/m²
Stream mass loading: 0 mg/m²
Includes upstream catchment
Data for project: Vines
Substance: 6_sw (1 application, vapour pressure = 3.78E-09 Pa)
Crop: Vines, late applns

Model


Manual Run-Off Reduction
Enter Run-off Mitigation Values
Enter values manually
Fractional reduction in run-off volume:
0
Fractional reduction in run-off flux:
0
Fractional reduction in erosion mass:
0
Fractional reduction in erosion flux:
0
Get using VFSmod
Filter strip buffer width:
4
m

WHICH MITIGATION?

- Anti-drift nozzles? No spray zones?
- Vegetated buffer?
- Hedgerows?
- High technology?

Step 4….Mitigation Measures

PEC air calculation

Pesticides in Air: Considerations for Exposure assessment (FOCUS, 2005).

- Tier 1: *trigger*.
  Vapour pressure lower than 10^{-5} Pa (20°C) for plants and 10^{-4} Pa (20°C) for soil

- Tier 2: modelling for the evaluation of residue deposition vs. distance from edge field.

- Tier 3: application of mitigation measurements to reduce PEC

GAP

Crop and/ or situation (a)	Country	Product name	F G or I (b)	Pests or Group of pests controlled (c)	Formulation Type (d-f)	Formulation Conc. of as (i)	Application method kind (f-h)	Application growth stage & season (j)	Application number min max (k)	Application interval between applications (min)	Application rate per treatment kg as/hL min max	Application rate per treatment water L/ha min max	Application rate per treatment kg as/ha min max	PHI (days) (l)	Remarks: (m)
Asparagus	Italy	Sencor SC	F	Weeds	SC	600	Broad-cast overall	BBCH 00 (pre-emergence)	1	-	0.070-0.140	300-500	0.35-0.42	60	
Carrots	Italy	Sencor SC	F	Weeds	SC	600	Spray	Post-emergence BBCH 13	1	-	0.035-0.081	300-500	0.175-0.245	60	
Potatoes	Italy	Sencor SC	F	Weeds	SC	600	Spraying	Pre-emergence	1		0.035-0.093	300-500	0.175-0.28	60	
								Post-emergence BBCH 12-51	3	14	0.140-0.233	300-500	0.07+ 0.07+ 0.07	60	
Soybean	Italy	Sencor	F	Annual broad-leaved weeds	SC	600	Spraying	Pre-emergence or Pre-seeding	1	-	0.042-0.070	300-500	0.210	-	
Tomatoes	Italy	Sencor SC	F	Annual broad-leaved weeds	SC	600	Broad-cast	Pre-seeding / pre planting	1		0.042-0.070	300-500	0.21	30	
								Post emergence/ post-transplanting	1		0,056-0,09		0.28		
									or 1+ 1	14	0,03-0,05		1° treatment 0,09-0,12 2° treatment 0,12-0,15		