

June 4-5th 2019

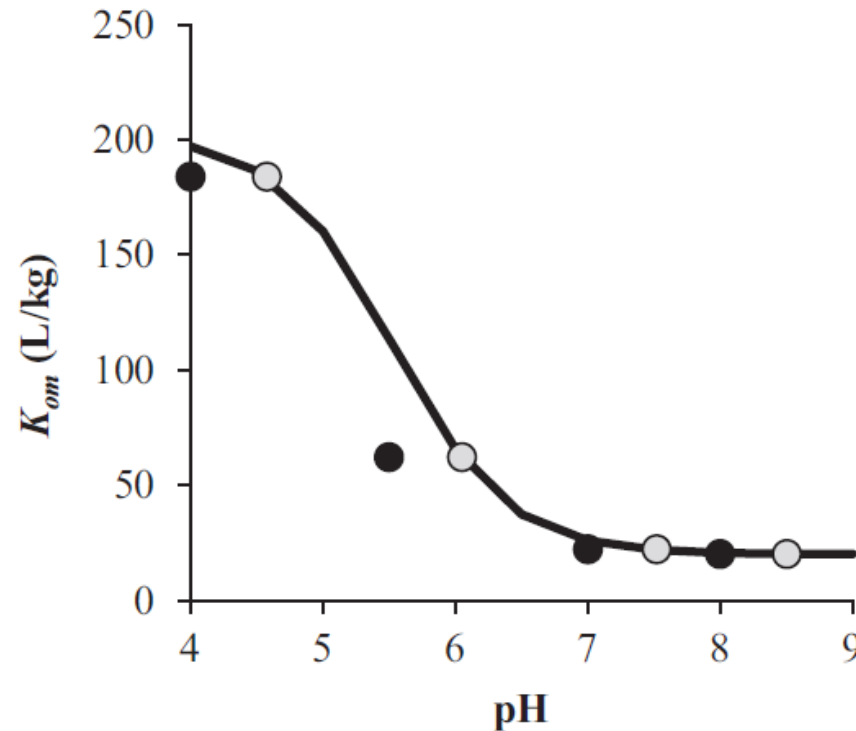
PERSAM Worked-examples: Soil pH dependent substances

Michael Klein

Trusted science for safe food

Example 7 (soil pH dependent substance)

1) Considering a pesticide that shows pH dependent sorption



EFSA (European Food Safety Authority), 2017. EFSA Guidance Document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil. EFSA Journal 2017;15(10):4982, 115 pp. <https://doi.org/10.2903/j.efsa.2017.4982>

Crop:

Maize

Number of applications:

2 application (2 * 1 kg/ha)

Type of application:

Spray application at BBCH 10-19 and BBCH 20-29

Time between applications:

14 days

G	Metabolite	
	M1	M2
300	200	100
0.1	90	90
10^{-8}	10^{-8}	10^{-8}
25	100	250
65.4	65.4	65.4
0.7	0.7	0.7
1,000	10	100
10^5	1,000	10^4
0.9	0.9	0.9
10	10	10
0.1	0.1	0.1
0	0	0
–	$0.7^{(h)}$	$1.0^{(i)}$

Substance properties:

Compound	Pesticide C
Molar mass (neutral form)	300 g/mol
Molar mass (anion)	299 g/mol
KOM (neutral form)	202.5 L/kg
KOM (anion)	20 L/kg
pKa	4.7
Δ pH	0.82
DegT50	250 d

G	Metabolite	
	M1	M2
300	200	100
0.1	90	90
10^{-8}	10^{-8}	10^{-8}
25	100	250
65.4	65.4	65.4
0.7	0.7	0.7
1,000	10	100
10^5	1,000	10^4
0.9	0.9	0.9
10	10	10
0.1	0.1	0.1
0	0	0
–	$0.7^{(h)}$	$1.0^{(i)}$

PERSAM 3.0.0-SNAPSHOT

PERSAM Graphical shell

Create a new project



PERSAM

v 3.0.0-SNAPSHOT

©2013-2019 developed by VITO <http://www.vito.be>

at the request of EFSA <http://www.efsa.eu>

[Refresh project tree](#)

New group...	New project...
Rename group...	Import project(s)...
Delete group...	Help

Batch queue status -- Queued: 0 Running: 0

[Cancel all calculations](#)

Tier 1. soil pH-dependent substances

At **Tier 1** soil incorporation is not taken into account

Create new project

Project name:

Output folder:

Select tier & substance type

Tier-1	Tier-2	Tier-3A
☒ Tier-1 Predefined scenarios for analytical model	☐ Tier-2 Crop-specific and substance-specific assessment based on a spatially distributed analytical model	☐ Tier-3A Crop-specific and substance-specific scenarios for numerical models

☒  Microbial active substances	☒  Other substances
---	---

- 1 - Tier & substance type

- 2 - Region

- 3 - Endpoints

- 4 - Crop

Regulatory zones

Create new project

Create new project

Help Cancel new project

Select zone(s) (multiple possible)



North
Central
South

- 1 -
Tier & substance type

- 2 -
Region

- 3 -
Endpoints

- 4 -
Crop

Previous Next

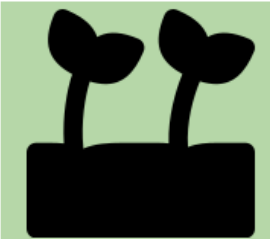
PECs selection

Create new project

Create new project

Help Cancel new project

Select endpoint(s) (multiple possible)



Concentration in total soil C_T

Concentration in pore water C_L

- 1 - Tier & substance type

- 2 - Region

- 3 - Endpoints

- 4 - Crop

Previous

Next

Crop type selection: at **Tier 1** only 2 options available



Create new project

Help Cancel new project

Select crop type

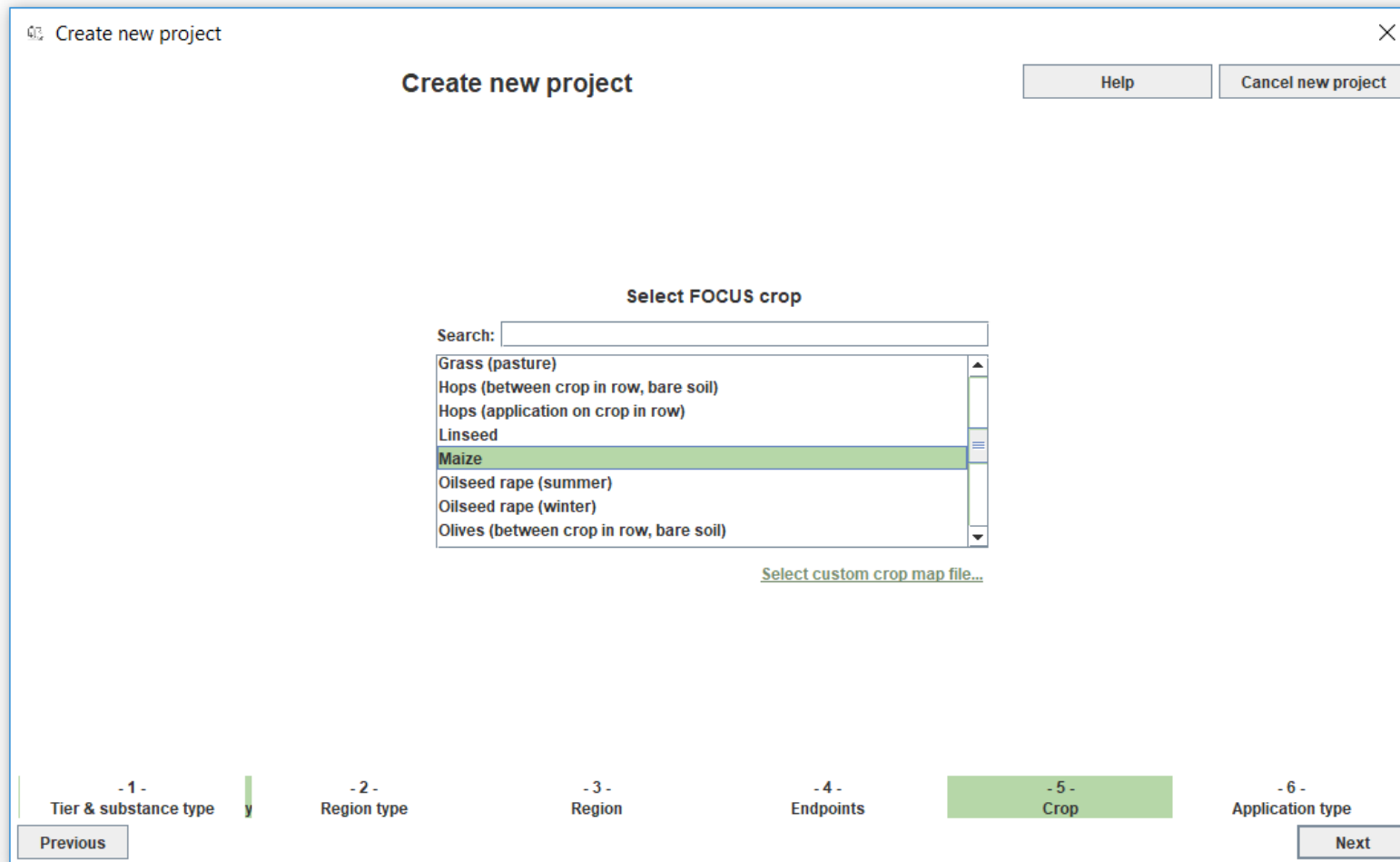
Annual crop Permanent crop

- 1 - Tier & substance type - 2 - Region - 3 - Endpoints - 4 - Crop

Previous Create ...

Tier 2. soil pH-dependent substances

Crop selection at **Tier 2 only**: FOCUS crops (annual and permanent) are available



Create new project

Help Cancel new project

Select FOCUS crop

Search:

- Grass (pasture)
- Hops (between crop in row, bare soil)
- Hops (application on crop in row)
- Linseed
- Maize**
- Oilseed rape (summer)
- Oilseed rape (winter)
- Olives (between crop in row, bare soil)

[Select custom crop map file...](#)

- 1 - Tier & substance type

- 2 - Region type

- 3 - Region

- 4 - Endpoints

- 5 - Crop

- 6 - Application type

Previous Next

Pesticide input parameters

 PERSAM 3.0.0-SNAPSHOT

 Soil-inc-case1-tier1 (595)

- Settings
- **Substances**
- Application scheme
- Fixed data

Click to add substance

Click to add substance

Click to add substance

Click to add substance

Click to add substance

Click to add substance

Click to add substance

Click to add substance

Click to add substance

Undo

Reset to defaults

Save

Key

Predefined

Custom

Sorption characteristics

PERSAM 3.0.0-SNAPSHOT

Soil-inc-case1-tier1 (595)

- Settings
- **Substances**
- Application scheme
- Fixed data

Substance configuration

Substance type

☐ Predefined substance ☒ Custom substance

substance 1

Substance properties

Code: Pesticide_C

K_{om} (mL/g): formula K_{oc} (L/kg): formula

DegT₅₀ (days): 250.0

M (g/mol): 300.0

E (kJ/mol): 65.4

Set custom formula Remove custom formula

Set custom formula Remove custom formula

Help Cancel OK Remove substance

Pesticide input parameters

PERSAM 3.0.0-SNAPSHOT

Soil-inc-case1-tier1 (595)

- Settings
- **Substances**
- Application scheme
- Fixed data

Define custom calculation

pH dependent sorption

pKa:	4.7	Δ pH:	0.82
M_{anion} (kg/mol):	299.0	$K_{\text{om,anion}}$ (m ³ /kg):	20.0
M_{acid} (kg/mol):	300.0	$K_{\text{om,acid}}$ (m ³ /kg):	202.5

Help Cancel OK

Pesticide input parameters

Degradation pathway (no metabolites considered)

PERSAM 3.0.0-SNAPSHOT

Soil-inc-case1-tier1 (595)

- Settings
- **Substances**
- Application scheme
- Fixed data

Pesticide A

Click to add substance

Click to add substance

Click to add substance

Click to add substance

Click to add substance

Click to add substance

Click to add substance

Click to add substance

Undo

Reset to defaults

Save

Key

Predefined

Custom

Application scheme

Two applications

At **Tier 1** crop interception is not taken into account

PERSAM 3.0.0-SNAPSHOT

Soil-inc-case1-tier1 (595)

- Settings
- Substances
- Application scheme
- Fixed data

rate (kg/ha)	dt (days)	Actions
1.0	0	
1.0	14	

Add application

application rate: ≥ 0 kg/ha

Time since first application (dt): 0 - 365 days

Add to table

Period of crop rotation

t_{cycle} : years

Application scheme

Two applications

At **Tier 2** crop interception is considered via the BBCH code

rate (kg/ha)	dt (days)	growth stage / season	Actions
1.0	0	BBCH 10-19	
1.0	14	BBCH 20-39	

Add application

application rate: ≥ 0 kg/ha

Time since first application (dt): 0 - 365 days

Crop development stage / season: ▼

Add to table

Period of crop rotation

t_{cycle} : ▼ years

Calculation



The calculation for this project is in progress.
Canceling will abort the calculation, and all project settings will be unlocked.

Cancel calculation

Model output Results of Tier 2

Select region

Central

Select endpoint

Concentration in total soil (mg/kg)

Tier-2 results

Plateau and peak concentrations

	default (5.0 cm)	z_{eco}
$C_{plateau}$	0.98	user
C_{peak}	10.63	

TWA concentrations

t_{avg}	default (5.0 cm)	z_{eco}
default (0 days)	10.63	user
user (1 days)	10.63	

PEC to RAC ratios

t_{avg}	default (5.0 cm)	z_{eco}
default (0 days)		user
user (1 days)		

Post-application concentrations

$t_{PostApp}$ (days)	30
z_{eco} (cm)	20.00
C_T (mg/kg)	5.48

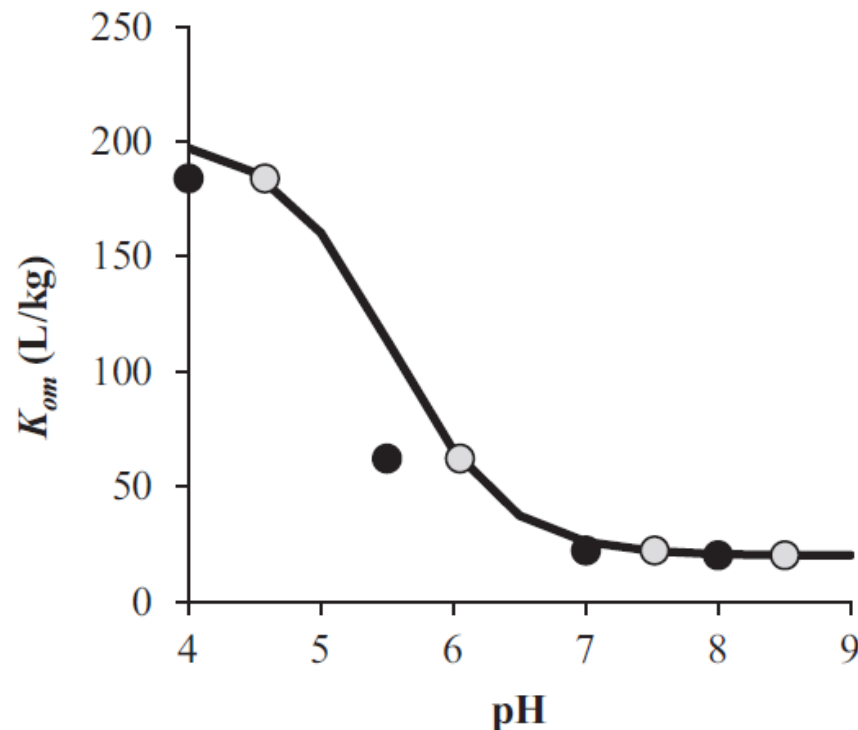
Tier-3A results

$z_{eco} = 5.0$ cm (default) Open transfer file Scenario locations

TIER 3A modelling is performed with PEARL and PELMO

FOCUS PELMO (vers.6.6.1) will be used in the following worked-example:

1) Concentration in total soil for the central zone



Tier 3A. soil pH-dependent substances

PERSAM generates a transfer file for Tier 3A assessment with PEARL and **PELMO**

PERSAM

Transfer file (.ptf)

soil-inc-case1-tier-2

- Settings
- Substances
- Application scheme
- Fixed data
- Results

Select region

North
Central
South

Select endpoint

Concentration in total soil (mg/kg)
Concentration in pore water (mg/L)

Tier-2 results

Plateau and peak concentrations

		default (5.0 cm)	user
C _{plateau}		1.08	
C _{peak}		4.01	

TWA concentrations

		default (5.0 cm)	user
t _{avg}			
default (0 days)		4.01	
user (21 days)		3.96	

PEC to RAC ratios

		default (5.0 cm)	user
t _{avg}			
default (0 days)			
user (21 days)			

Post-application concentrations

t _{PostApp} (days)	0
z _{eco} (cm)	20.00
C _T (mg/kg)	4.40

Tier-3A results

z_{eco} = 5.0 cm (default)

Open transfer file

Scenario locations

Open Tier-3A PDF report

Open Tier-2 PDF report

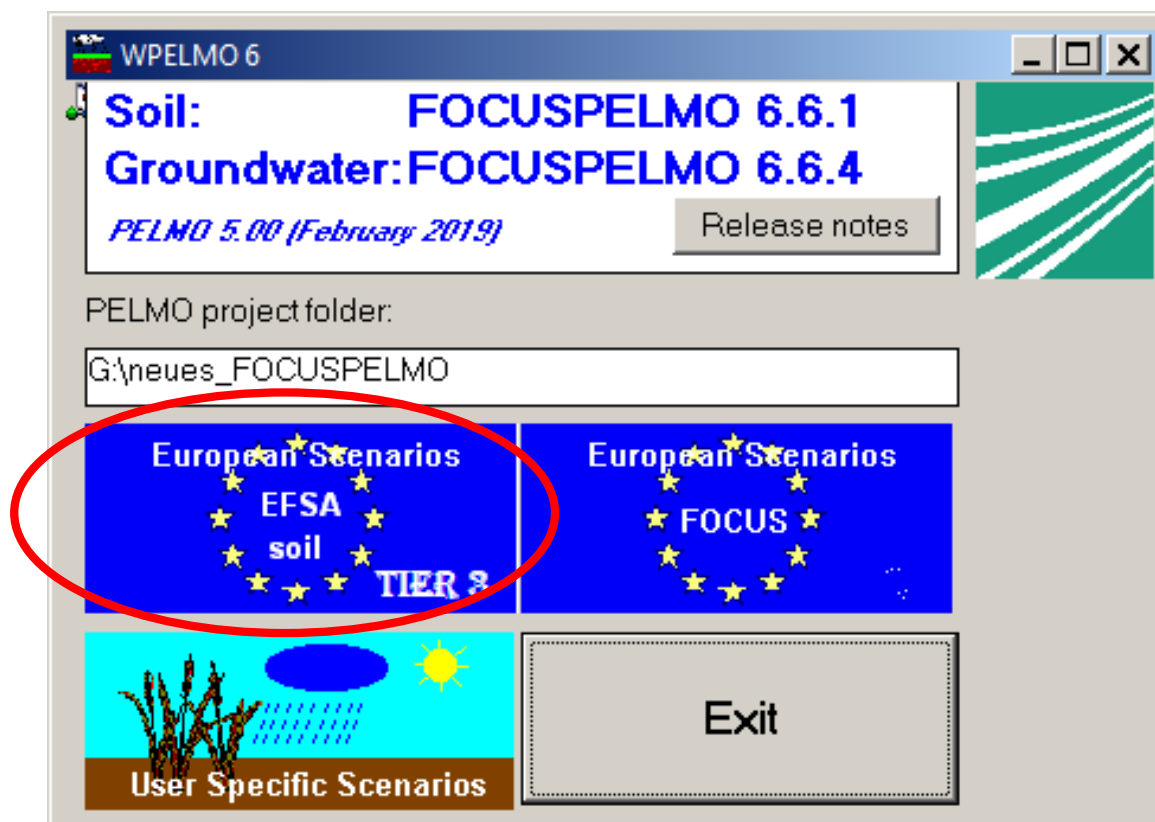


```
* PERSAM Transfer file
* Generated on 27/05/2019, 16:10
*
North RegZone Regulatory zone (options: North, Centre, South)
TotSoil TypeOfREP Type of endpoint (options: TotSoil, PoreWat)
3844, 1745 Location X/Y coordinates
P Substance Substance assessed (options: P, M1A, M1B, M1C, M1D, M2A, M2B, M2C, M2D)
1.00 Ref (-) Refinement factor for final PEC
16 PERSAMCropNo PERSAM crop number
Coarse Soil TypeOfSoil Soil texture (options: Coarse, Medium, MediumFine, Fine, VeryFine, Organic)
0.12 CntOnSCa (kg.kg-1) Topsoil organic matter content
4.40 pHtp (-) Topsoil pH
647.00 Pro (mm) Mean annual precipitation
8.00 Temp (C) Mean annual temperature
Pesticide A Name, P Substance name
-99 Name, M1A -----II-----
-99 Name, M1B -----II-----
-99 Name, M1C -----II-----
-99 Name, M1D -----II-----
-99 Name, M2A -----II-----
-99 Name, M2B -----II-----
-99 Name, M2C -----II-----
-99 Name, M2D -----II-----
300.00 MolMas, P (g.mol-1) Molar mass
-99 MolMas, M1A (g.mol-1) -----II-----
-99 MolMas, M1B (g.mol-1) -----II-----
-99 MolMas, M1C (g.mol-1) -----II-----
-99 MolMas, M1D (g.mol-1) -----II-----
-99 MolMas, M2A (g.mol-1) -----II-----
-99 MolMas, M2B (g.mol-1) -----II-----
-99 MolMas, M2C (g.mol-1) -----II-----
-99 MolMas, M2D (g.mol-1) -----II-----
-99 P -> M1A (-) Molar formation fraction
-99 P -> M1B (-) -----II-----
-99 P -> M1C (-) -----II-----
-99 P -> M1D (-) -----II-----
-99 M1A -> M2A (-) -----II-----
-99 M1A -> M2B (-) -----II-----
-99 M1A -> M2C (-) -----II-----
-99 M1A -> M2D (-) -----II-----
-99 M1B -> M2A (-) -----II-----
-99 M1B -> M2B (-) -----II-----
-99 M1B -> M2C (-) -----II-----
-99 M1B -> M2D (-) -----II-----
-99 M1C -> M2A (-) -----II-----
-99 M1C -> M2B (-) -----II-----
-99 M1C -> M2C (-) -----II-----
-99 M1C -> M2D (-) -----II-----
-99 M1D -> M2A (-) -----II-----
-99 M1D -> M2B (-) -----II-----
-99 M1D -> M2C (-) -----II-----
-99 M1D -> M2D (-) -----II-----
250.00 DT50Ref, P (d) Half-life time
-99 DT50Ref, M1A (d) -----II-----
-99 DT50Ref, M1B (d) -----II-----
-99 DT50Ref, M1C (d) -----II-----
-99 DT50Ref, M1D (d) -----II-----
-99 DT50Ref, M2A (d) -----II-----
-99 DT50Ref, M2B (d) -----II-----
-99 DT50Ref, M2C (d) -----II-----
-99 DT50Ref, M2D (d) -----II-----
65.40 MolEntTra, P (kJ.mol-1) Molar activation energy
-99 MolEntTra, M1A (kJ.mol-1) -----II-----
-99 MolEntTra, M1B (kJ.mol-1) -----II-----
-99 MolEntTra, M1C (kJ.mol-1) -----II-----
-99 MolEntTra, M1D (kJ.mol-1) -----II-----
-99 MolEntTra, M2A (kJ.mol-1) -----II-----
-99 MolEntTra, M2B (kJ.mol-1) -----II-----
-99 MolEntTra, M2C (kJ.mol-1) -----II-----
-99 MolEntTra, M2D (kJ.mol-1) -----II-----
1000.00 KorEq, P (L.kg-1) Coef. eq. sorption on org. matter
-99 KorEq, M1A (L.kg-1) -----II-----
-99 KorEq, M1B (L.kg-1) -----II-----
-99 KorEq, M1C (L.kg-1) -----II-----
-99 KorEq, M1D (L.kg-1) -----II-----
-99 KorEq, M2A (L.kg-1) -----II-----
-99 KorEq, M2B (L.kg-1) -----II-----
-99 KorEq, M2C (L.kg-1) -----II-----
-99 KorEq, M2D (L.kg-1) -----II-----
0 ZEAOTop (m) Top of the evaluation depth
0.50 ZEAObot (m) Bottom of the evaluation depth
1 DefIntExt (d) Repeat interval of events (options: 1, 2, 3)
0 IntPostApp (d) Time interval for post-application PEC (days after last application)
AppSoftT OptApp Application (options: AppCpUser, AppSolnT, AppSolTI)
10.00 ZApp (mg) Application depth (incorporation or injection)
1 NApp (-) Number of applications events
* Application table (day - rate (kg.ha-1) - crop interception (fraction of dosage, dimensionless))
table Applications
0
end_table
1.00
0
```



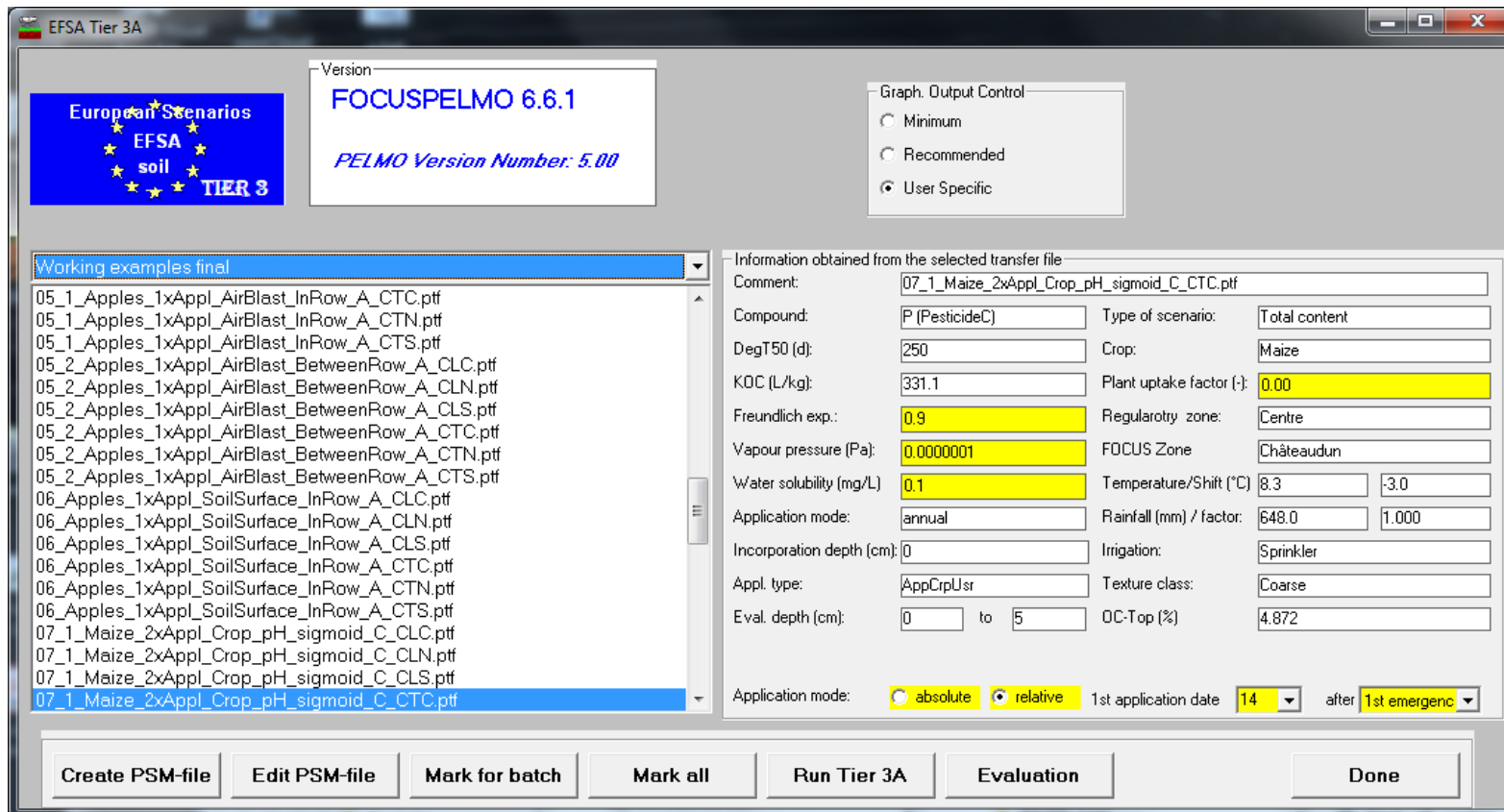
PELMO

PELMO Graphical shell



Scenario refinement with PELMO

Further substance properties are required at **Tier 3 A**
Time of application is considered at **Tier 3 A** and will affect water balance



EFSA Tier 3A

Version: FOCUSPELMO 6.6.1
PELMO Version Number: 5.00

Graph. Output Control
☐ Minimum
☐ Recommended
☒ User Specific

Working examples final

- 05_1_Apples_1xAppl_AirBlast_InRow_A_CTC.ptf
- 05_1_Apples_1xAppl_AirBlast_InRow_A_CTN.ptf
- 05_1_Apples_1xAppl_AirBlast_InRow_A_CTS.ptf
- 05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CLC.ptf
- 05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CLN.ptf
- 05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CLS.ptf
- 05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CTC.ptf
- 05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CTN.ptf
- 05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CTS.ptf
- 06_Apples_1xAppl_SoilSurface_InRow_A_CLC.ptf
- 06_Apples_1xAppl_SoilSurface_InRow_A_CLN.ptf
- 06_Apples_1xAppl_SoilSurface_InRow_A_CLS.ptf
- 06_Apples_1xAppl_SoilSurface_InRow_A_CTC.ptf
- 06_Apples_1xAppl_SoilSurface_InRow_A_CTN.ptf
- 06_Apples_1xAppl_SoilSurface_InRow_A_CTS.ptf
- 07_1_Maize_2xAppl_Crop_pH_sigmoid_C_CLC.ptf
- 07_1_Maize_2xAppl_Crop_pH_sigmoid_C_CLN.ptf
- 07_1_Maize_2xAppl_Crop_pH_sigmoid_C_CLS.ptf
- 07_1_Maize_2xAppl_Crop_pH_sigmoid_C_CTC.ptf

Information obtained from the selected transfer file

Comment: 07_1_Maize_2xAppl_Crop_pH_sigmoid_C_CTC.ptf

Compound: P (PesticideC) Type of scenario: Total content

DegT50 (d): 250 Crop: Maize

KOC (L/kg): 331.1 Plant uptake factor (-): 0.00

Freundlich exp.: 0.9 Regularity zone: Centre

Vapour pressure (Pa): 0.0000001 FOCUS Zone: Châteaudun

Water solubility (mg/L): 0.1 Temperature/Shift (°C): 8.3 -3.0

Application mode: annual Rainfall (mm) / factor: 648.0 1.000

Incorporation depth (cm): 0 Irrigation: Sprinkler

Appl. type: AppCrpUst Texture class: Coarse

Eval. depth (cm): 0 to 5 OC-Top (%): 4.872

Application mode: ☐ absolute ☒ relative 1st application date: 14 after 1st emergenc

Create PSM-file Edit PSM-file Mark for batch Mark all Run Tier 3A Evaluation Done

Tier 3A with PELMO: soil pH-dependent substances

EFSA Tier 3A

Version: **FOCUSPELMO 6.6.1**
PELMO Version Number: 5.00

Graph. Output Control
☐ Minimum
☐ Recommended
☒ User Specific

Working examples final

- 05_1_Apples_1xAppl_AirBlast_InRow_A_CTC.ptf
- 05_1_Apples_1xAppl_AirBlast_InRow_A_CTN.ptf
- 05_1_Apples_1xAppl_AirBlast_InRow_A_CTS.ptf
- 05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CLC.ptf
- 05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CLN.ptf
- 05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CLS.ptf
- 05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CTC.ptf
- 05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CTN.ptf
- 05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CTS.ptf
- 06_Apples_1xAppl_SoilSurface_InRow_A_CLC.ptf
- 06_Apples_1xAppl_SoilSurface_InRow_A_CLN.ptf
- 06_Apples_1xAppl_SoilSurface_InRow_A_CLS.ptf
- 06_Apples_1xAppl_SoilSurface_InRow_A_CTC.ptf
- 06_Apples_1xAppl_SoilSurface_InRow_A_CTN.ptf
- 06_Apples_1xAppl_SoilSurface_InRow_A_CTS.ptf
- 07_1_Maize_2xAppl_Crop_pH_sigmoid_C_CLC.ptf
- 07_1_Maize_2xAppl_Crop_pH_sigmoid_C_CLN.ptf
- 07_1_Maize_2xAppl_Crop_pH_sigmoid_C_CLS.ptf
- 07_1_Maize_2xAppl_Crop_pH_sigmoid_C_CTC.ptf

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Vapour pressure (Pa): 0.0000001 FOCUS Zone: Châteaudun

Water solubility (mg/L): 0.1 Temperature/Shift (°C): 8.3 -3.0

Application mode: annual Rainfall (mm) / factor: 648.0 1.000

Incorporation depth (cm): 0 Irrigation: Sprinkler

Appl. type: AppCpUsr Texture class: Coarse

Eval. depth (cm): 0 to 5 OC-Top (%): 4.872

Application mode: ☒ absolute ☒ relative 1st application date: 14 after 1st emergenc

Create PSM-file Edit PSM-file Mark for batch Mark all Run Tier 3A Evaluation Done

Tier 3A with PELMO: soil pH-dependent substances

EFSA Tier 3A

Version: **FOCUSPELMO 6.6.1**
PELMO Version Number: 5.00

Graph. Output Control
☐ Minimum
☐ Recommended
☒ User Specific

Working examples final

- 05_1_Apples_1xAppl_AirBlast_InRow_A_CTC.ptf
- 05_1_Apples_1xAppl_AirBlast_InRow_A_CTN.ptf
- 05_1_Apples_1xAppl_AirBlast_InRow_A_CTS.ptf
- 05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CLC.ptf
- 05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CLN.ptf
- 05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CLS.ptf
- 05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CTC.ptf
- 05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CTN.ptf
- 05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CTS.ptf
- 06_Apples_1xAppl_SoilSurface_InRow_A_CLC.ptf
- 06_Apples_1xAppl_SoilSurface_InRow_A_CLN.ptf
- 06_Apples_1xAppl_SoilSurface_InRow_A_CLS.ptf
- 06_Apples_1xAppl_SoilSurface_InRow_A_CTC.ptf
- 06_Apples_1xAppl_SoilSurface_InRow_A_CTN.ptf
- 06_Apples_1xAppl_SoilSurface_InRow_A_CTS.ptf
- 07_1_Maize_2xAppl_Crop_pH_sigmoid_C_CLC.ptf
- 07_1_Maize_2xAppl_Crop_pH_sigmoid_C_CLN.ptf
- 07_1_Maize_2xAppl_Crop_pH_sigmoid_C_CLS.ptf
- 07_1_Maize_2xAppl_Crop_pH_sigmoid_C_CTC.ptf

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Vapour pressure (Pa): 0.0000001 FOCUS Zone: Châteaudun

Water solubility (mg/L): 0.1 Temperature/Shift (°C) 8.3 -3.0

Application mode: annual Rainfall (mm) / factor: 648.0 1.000

Incorporation depth (cm): 0 Irrigation: Sprinkler

Appl. type: AppCpUsr Texture class: Coarse

Eval. depth (cm): 0 to 5 OC-Top (%) 4.872

Application mode: ☒ absolute ☒ relative 1st application date 14 after 1st emergenc

Create PSM-file Edit PSM-file **Mark for batch** Mark all Run Tier 3A Evaluation Done

Tier 3A with PELMO: soil pH-dependent substances

EFSA Tier 3A

Version: **FOCUSPELMO 6.6.1**
PELMO Version Number: 5.00

European Scenarios
EFSA
soil
TIER 3

Graph. Output Control
☐ Minimum
☐ Recommended
☒ User Specific

Working examples final

05_1_Apples_1xAppl_AirBlast_InRow_A_CTC.ptf
05_1_Apples_1xAppl_AirBlast_InRow_A_CTN.ptf
05_1_Apples_1xAppl_AirBlast_InRow_A_CTS.ptf
05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CLC.ptf
05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CLN.ptf
05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CLS.ptf
05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CTC.ptf
05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CTN.ptf
05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CTS.ptf
06_Apples_1xAppl_SoilSurface_InRow_A_CLC.ptf
06_Apples_1xAppl_SoilSurface_InRow_A_CLN.ptf
06_Apples_1xAppl_SoilSurface_InRow_A_CLS.ptf
06_Apples_1xAppl_SoilSurface_InRow_A_CTC.ptf
06_Apples_1xAppl_SoilSurface_InRow_A_CTN.ptf
06_Apples_1xAppl_SoilSurface_InRow_A_CTS.ptf
07_1_Maize_2xAppl_Crop_pH_sigmoid_C_CLC.ptf
07_1_Maize_2xAppl_Crop_pH_sigmoid_C_CLN.ptf
07_1_Maize_2xAppl_Crop_pH_sigmoid_C_CLS.ptf
07_1_Maize_2xAppl_Crop_pH_sigmoid_C_CTC.ptf

Information obtained from the selected transfer file

Comment: 07_1_Maize_2xAppl_Crop_pH_sigmoid_C_CTC.ptf

Compound: P (PesticideC) Type of scenario: Total content

DegT50 (d): 250 Crop: Maize

KOC (L/kg): 331.1 Plant uptake factor (-): 0.00

Freundlich exp.: 0.9 Regularotry zone: Centre

Vapour pressure (Pa): 0.0000001 FOCUS Zone: Châteaudun

Water solubility (mg/L): 0.1 Temperature/Shift (°C) 8.3 -3.0

Application mode: annual Rainfall (mm) / factor: 648.0 1.000

Incorporation depth (cm): 0 Irrigation: Sprinkler

Appl. type: AppCpUsr Texture class: Coarse

Eval. depth (cm): 0 to 5 OC-Top (%): 4.872

Application mode: ☐ absolute ☒ relative 1st application date 14 after 1st emergenc

Create PSM-file Edit PSM-file Mark for batch Mark all **Run Tier 3A** Evaluation Done

Tier 3A with PELMO: soil pH-dependent substances

EFSA Tier 3A

Version: **FOCUSPELMO 6.6.1**
PELMO Version Number: 5.00

Graph. Output Control
☐ Minimum
☐ Recommended
☒ User Specific

Working examples final

- 05_1_Apples_1xAppl_AirBlast_InRow_A_CTC.ptf
- 05_1_Apples_1xAppl_AirBlast_InRow_A_CTN.ptf
- 05_1_Apples_1xAppl_AirBlast_InRow_A_CTS.ptf
- 05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CLC.ptf
- 05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CLN.ptf
- 05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CLS.ptf
- 05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CTC.ptf
- 05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CTN.ptf
- 05_2_Apples_1xAppl_AirBlast_BetweenRow_A_CTS.ptf
- 06_Apples_1xAppl_SoilSurface_InRow_A_CLC.ptf
- 06_Apples_1xAppl_SoilSurface_InRow_A_CLN.ptf
- 06_Apples_1xAppl_SoilSurface_InRow_A_CLS.ptf
- 06_Apples_1xAppl_SoilSurface_InRow_A_CTC.ptf
- 06_Apples_1xAppl_SoilSurface_InRow_A_CTN.ptf
- 06_Apples_1xAppl_SoilSurface_InRow_A_CTS.ptf
- 07_1_Maize_2xAppl_Crop_pH_sigmoid_C_CLC.ptf
- 07_1_Maize_2xAppl_Crop_pH_sigmoid_C_CLN.ptf
- 07_1_Maize_2xAppl_Crop_pH_sigmoid_C_CLS.ptf
- 07_1_Maize_2xAppl_Crop_pH_sigmoid_C_CTC.ptf

Information obtained from the selected transfer file

Comment: 07_1_Maize_2xAppl_Crop_pH_sigmoid_C_CTC.ptf

Compound: P (PesticideC) Type of scenario: Total content

DegT50 (d): 250 Crop: Maize

KOC (L/kg): 331.1 Plant uptake factor (-): 0.00

Freundlich exp.: 0.9 Regularotry zone: Centre

Vapour pressure (Pa): 0.0000001 FOCUS Zone: Châteaudun

Water solubility (mg/L): 0.1 Temperature/Shift (°C): 8.3 -3.0

Application mode: annual Rainfall (mm) / factor: 648.0 1.000

Incorporation depth (cm): 0 Irrigation: Sprinkler

Appl. type: AppCpUsr Texture class: Coarse

Eval. depth (cm): 0 to 5 OC-Top (%): 4.872

Application mode: ☐ absolute ☒ relative 1st application date: 14 after 1st emergenc

Create PSM-file Edit PSM-file Mark for batch Mark all Run Tier 3A **Evaluation** Done

Results of Tier 3 with PELMO

Evaluation of Simulation (EFSA persistence in soil)

Results of PERSAM Tier 3

Project: Working examples final Scenario Type: total content

PT-File: 07_1_Maize_2xAppl_Crop_pH_sigmoid_C_CTC

Crop: Maize ERD (cm): 5

Regulatory zone: Centre FOCUS-zone: Châteaudun beginning at: 0

Temp shift (°C): -3.000 Rain factor: 1.000 OC (%): 4.87

Show tabular output

Echo **PEC soil** Mass Balance Summary

Create Diagrams (Daily Time Step)

Total content in soil at 1 cm for Active Substance

☐ Cumulative from: January 33

☒ Non-cumulative to: December 52

Show Diagram

Done

Tier 3A with PELMO: soil pH-dependent substances

PECs in soil for Central Europe following spray application of compound C

Table of actual and time weighted average concentrations in soil

Tier 3A simulation:

*** FOCUS PELMO 6. 6. 1 *** (PELMO 5.0)
 Compound: 07_1_Maize_2xAppl_Crop_pH_sigmoid_C CTC
 Soil: Coarse (4.87% OC)
 Crop: Ver 1 Châteaudun, maize
 Climate: Ver 1 Châteaudun scenario (48.05 N, 1.38 E)) Year:11
 Scenario type: Total content
 Begin of the evaluation depth (cm): 0

Substance: P (PesticideC)

TWA (d)	PEC (mg/kg)	Begin TWA (d)
0	4.9867600	1 June 38
1	4.9867600	1 June 38
2	4.9851400	31 May 38
3	4.9826400	31 May 38
4	4.9807700	31 May 38
7	4.9690600	31 May 38
14	4.9352600	31 May 38
21	4.8944086	31 May 38
28	4.8501521	31 May 38
56	4.6181675	29 May 38
100	4.1905882	29 May 35
Plateau (20 cm)	1.7379600	29 May 38
Conc. after 90 d	2.0895500	27 August 50
Conc. after 120 d	1.9807100	26 September 50
Conc. after 165 d	1.8855850	10 November 50
Conc. after 200 d	1.8223350	15 December 50
Conc. after 270 d	1.7586650	23 February 51
Conc. after 320 d	1.7052000	14 April 51
Conc. after 365 d	1.6763200	29 May 51

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Tier	PECmax (TWA=0)
1 (PERSAM)	-
2 (PERSAM)	10.63
3 (PELMO)	4.99



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