

June 4-5th 2019

PERSAM Worked-examples: Use of the guidance for metabolites

Michael Klein

Trusted science for safe food

Example 9 (parent and metabolites)

- 1) Considering a pesticide together with two sequential metabolites
- 2) Substance of concern Metabolite M2

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

Substance properties:

	Pesticide G	Metabolite M1	Metabolite M2
DegT50 (d)	25	100	250
KOM (L/kg)	1000	10	100
Molar mass	300	200	100
Formation fraction	-	0.7	1.0

	Metabolite	
G	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](#)

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
Predefined scenarios for analytical model	Crop-specific and substance-specific assessment based on a spatially distributed analytical model	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

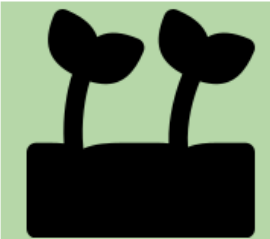
PECs selection

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

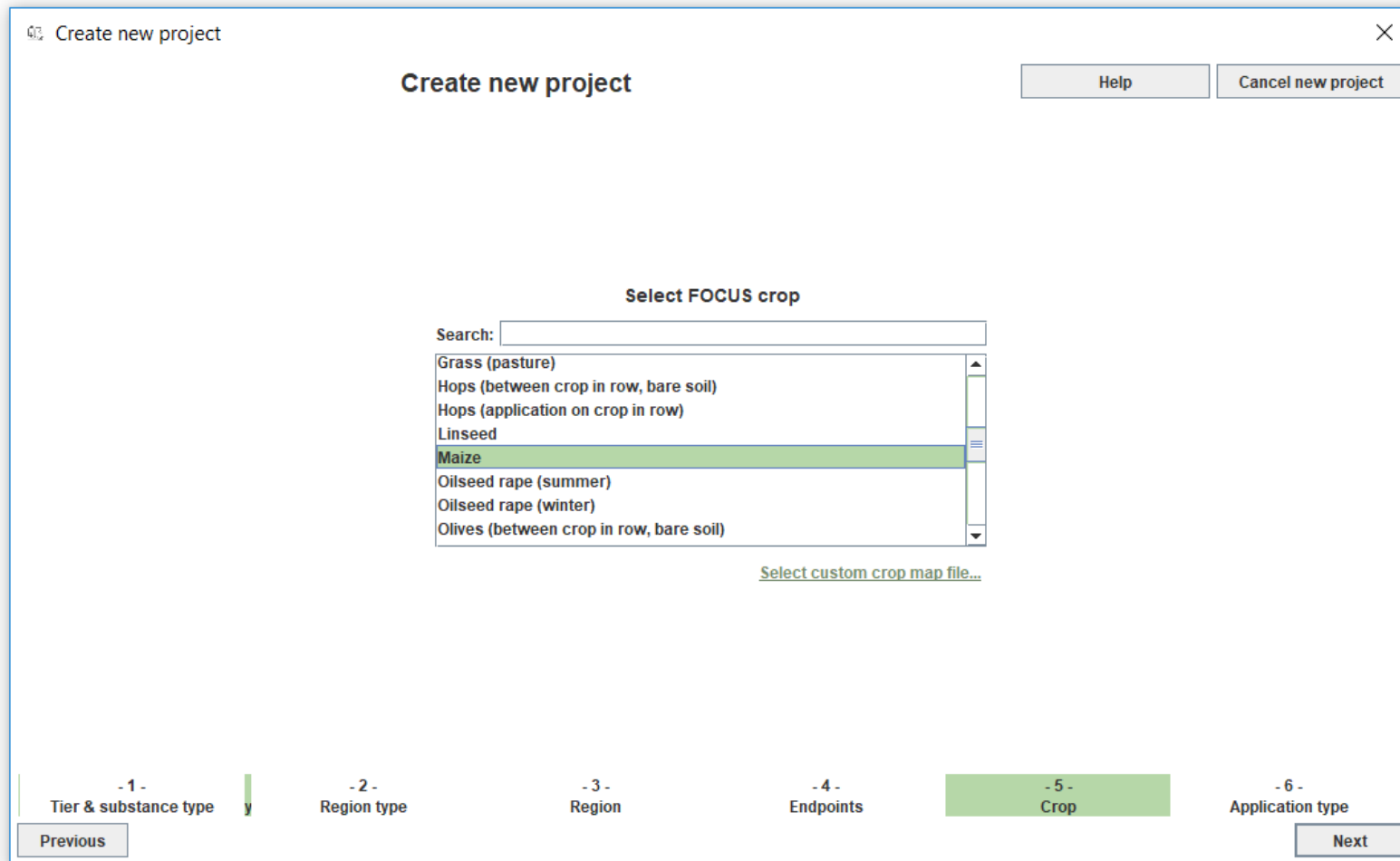
Next

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



The screenshot shows a software window titled "Create new project" with a close button (X) in the top right corner. Below the title bar, there are two buttons: "Help" and "Cancel new project". The main area of the window is titled "Select crop type" and contains two options: "Annual crop" (represented by a green square with a circular arrow icon) and "Permanent crop" (represented by a black infinity symbol). The "Annual crop" option is highlighted with a red circle. At the bottom of the window, there is a progress bar with four steps: "- 1 - Tier & substance type", "- 2 - Region", "- 3 - Endpoints", and "- 4 - Crop". The "- 4 - Crop" step is highlighted in green and has a "Create ..." button next to it, which is also circled in red. A "Previous" button is located at the bottom left.

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

Pesticide input parameters

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: Substance_G

K_{om} (mL/g): 1000.0 K_{oc} (L/kg): 1724.00

DegT₅₀ (days): 25.0

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

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

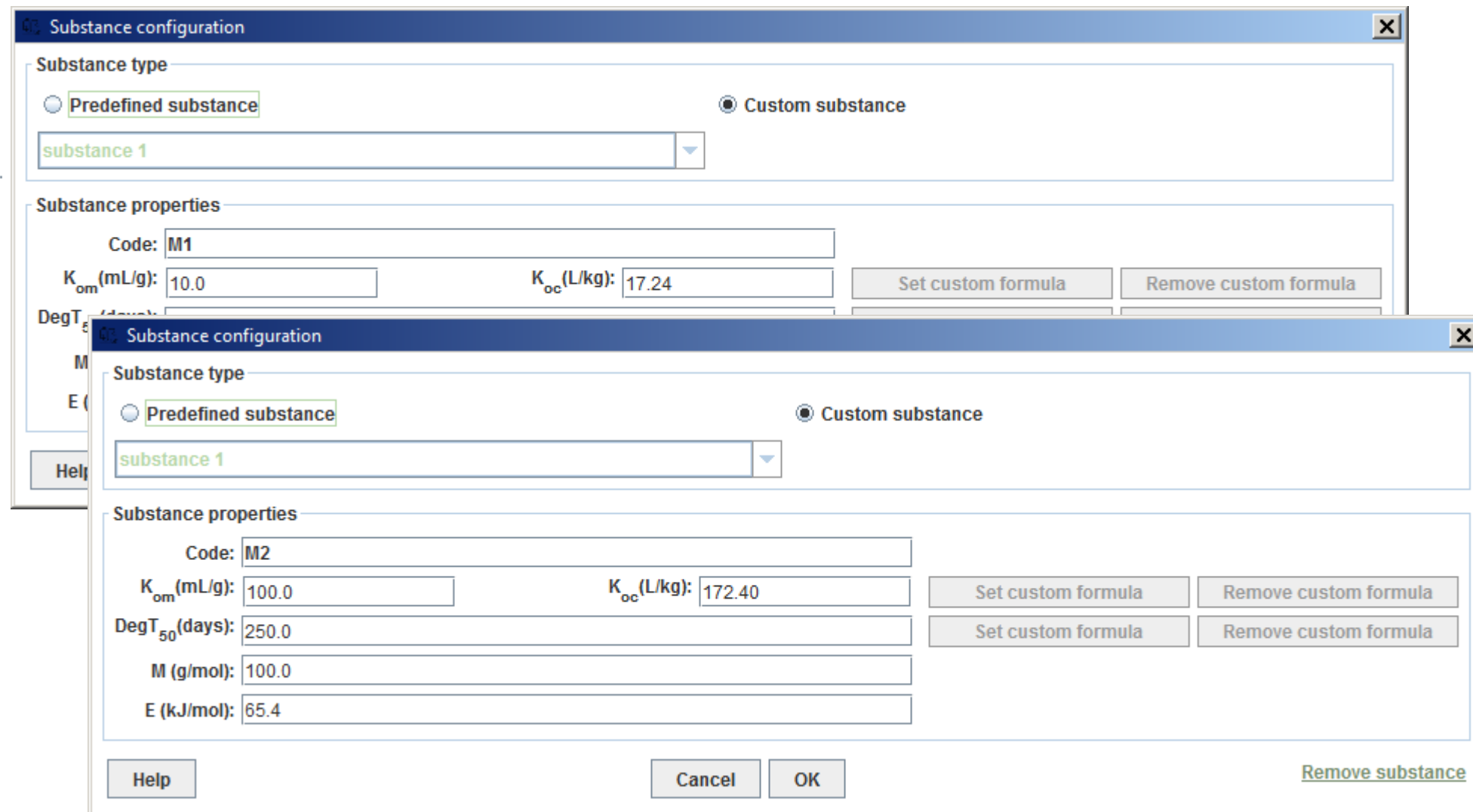
Custom

Metabolite input parameters

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: M1

K_{om} (mL/g): 10.0 K_{oc} (L/kg): 17.24

[Set custom formula](#) [Remove custom formula](#)

Substance configuration

Substance type

☐ Predefined substance ☒ Custom substance

substance 1

Substance properties

Code: M2

K_{om} (mL/g): 100.0 K_{oc} (L/kg): 172.40

DegT₅₀ (days): 250.0

M (g/mol): 100.0

E (kJ/mol): 65.4

[Set custom formula](#) [Remove custom formula](#)

[Set custom formula](#) [Remove custom formula](#)

[Help](#) [Cancel](#) [OK](#) [Remove substance](#)

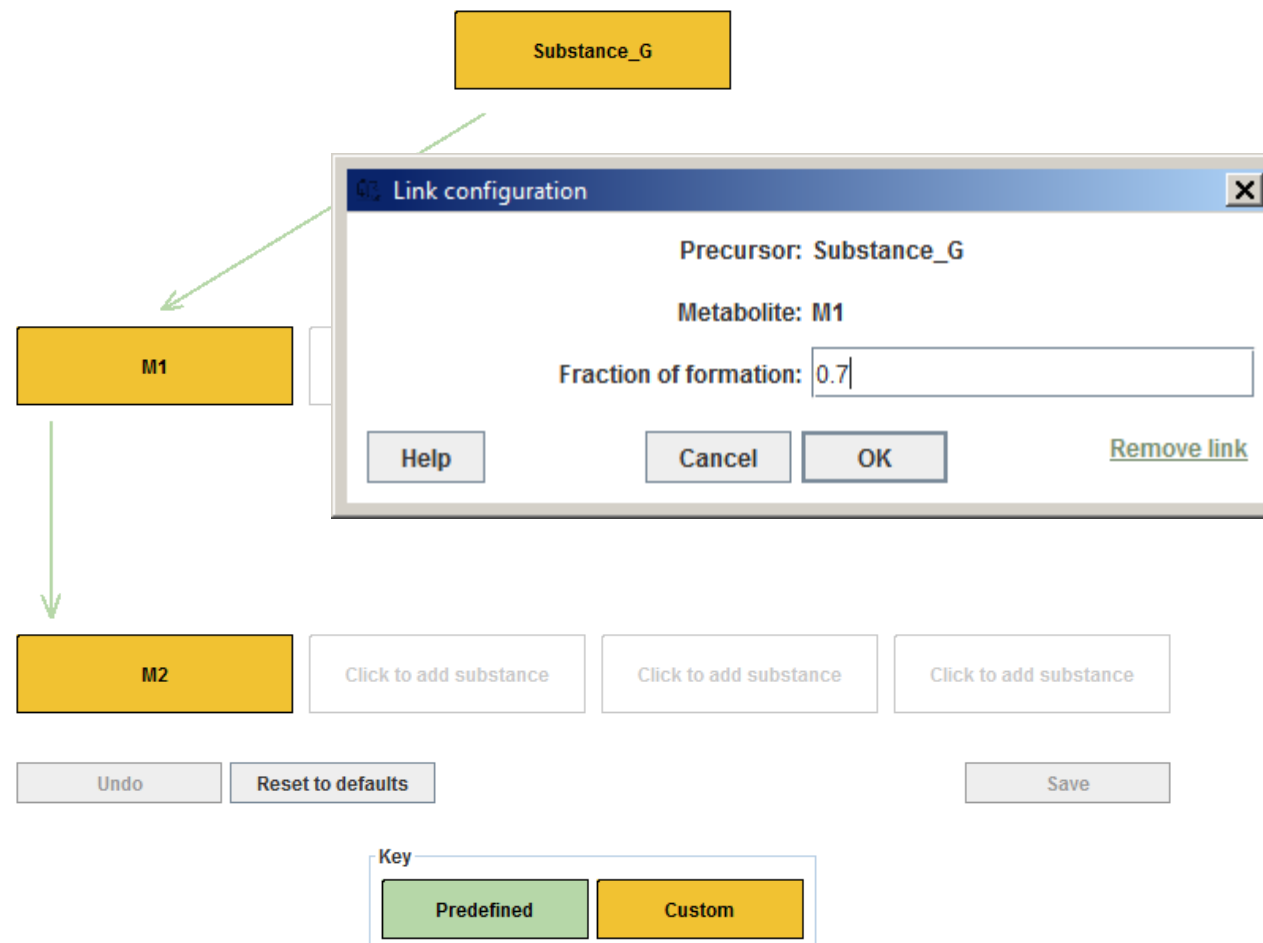
Formation fractions

PERSAM project: Metabolite Tier 1 (610)

PERSAM 3.0.0-SNAPSHOT

Soil-inc-case1-tier1 (595)

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



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 1 (left) and Tier 2 (right) for metabolite M2

Select region

Central

Select endpoint

Concentration in total soil (mg/kg)

Tier-1 results

Plateau and peak concentrations

	default (5.0 cm)	user
$C_{plateau}$	0.51	
C_{peak}	4.68	

TWA concentrations

	default (5.0 cm)	user
t_{avg}		
default (0 days)	4.68	
user (1 days)	4.68	

PEC to RAC ratios

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

Post-application concentrations

$t_{PostApp}$ (days)	0
Z_{eco} (cm)	20.00
C_T (mg/kg)	2.65

Tier-2 results

Plateau and peak concentrations

	default (5.0 cm)	user
$C_{plateau}$	0.13	
C_{peak}	2.42	

TWA concentrations

	default (5.0 cm)	user
t_{avg}		
default (0 days)	2.42	
user (1 days)	2.42	

PEC to RAC ratios

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

Post-application concentrations

$t_{PostApp}$ (days)	30
Z_{eco} (cm)	20.00
C_T (mg/kg)	1.19

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
- 2) Substance of concern: M2

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_r (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



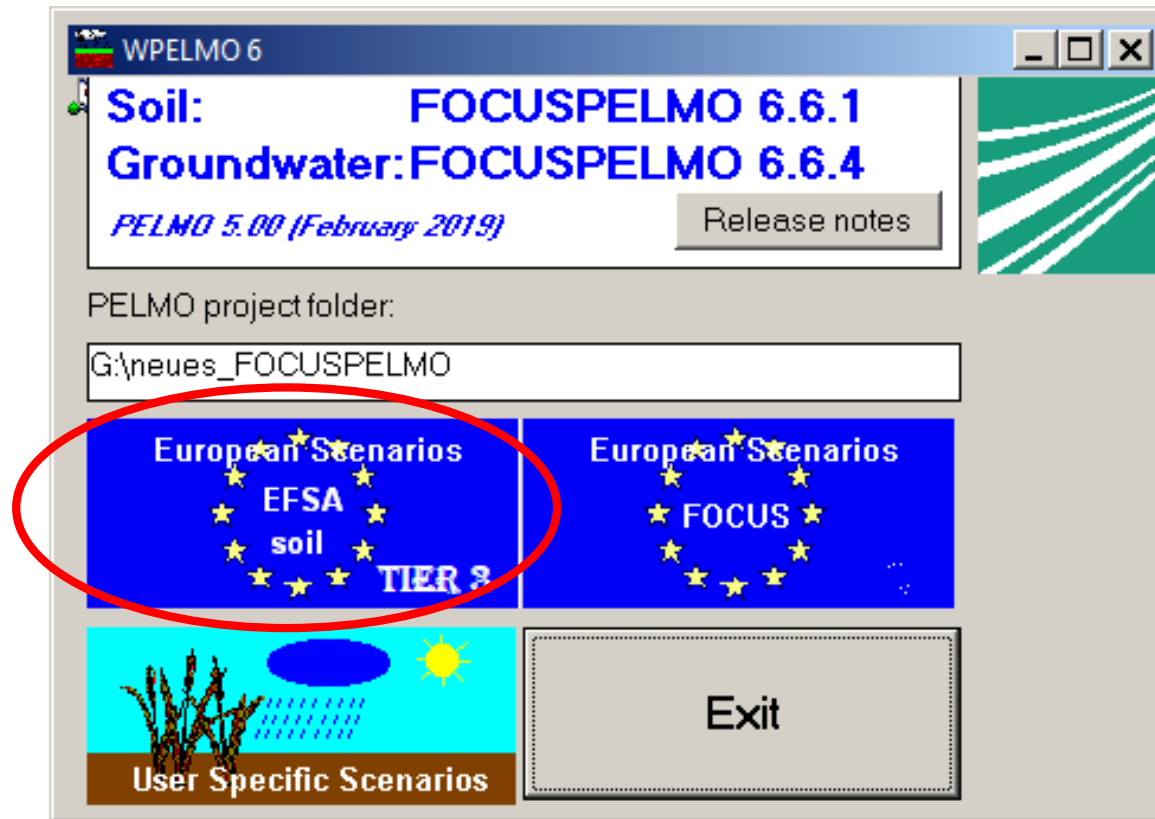
```

* PERSAM Transfer file
* Generated on 27/05/2019, 16:10
*
North RegZone Regulatory zone (options: North, Centre, South)
TotSoil TypePREP 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 SoilTypeD 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 DelTmExt (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, AppSolnI)
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
  
```



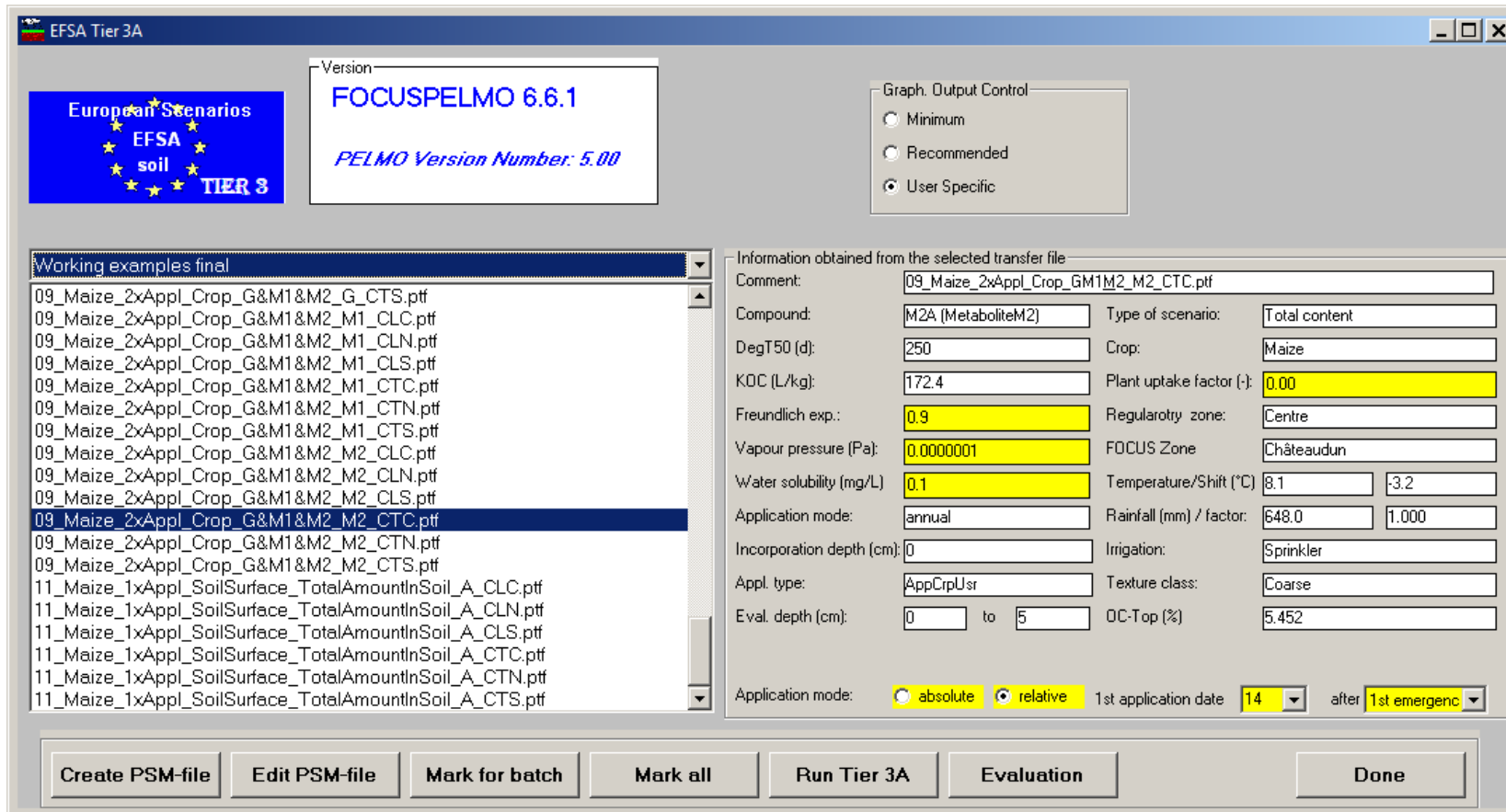
PELMO

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



The screenshot displays the EFSA Tier 3A software interface. The title bar reads "EFSA Tier 3A". On the left, there is a logo for "European Scenarios EFSA soil TIER 3". The main area is divided into several sections:

- Version:** FOCUSPELMO 6.6.1
PELMO Version Number: 5.00
- Graph. Output Control:** Minimum, Recommended, User Specific (selected).
- Working examples final:** A list of files including various scenarios for Maize and Soil Surface Total Amount in Soil (A, CLC, CLN, CLS, CTC, CTN).
- Information obtained from the selected transfer file:**
 - Comment: 09_Maize_2xAppl_Crop_GM1M2_M2_CTC.ptf
 - Compound: M2A (MetaboliteM2)
 - Type of scenario: Total content
 - DegT50 (d): 250
 - Crop: Maize
 - KOC (L/kg): 172.4
 - 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): 8.1, -3.2
 - Application mode: annual
 - Rainfall (mm) / factor: 648.0, 1.000
 - Incorporation depth (cm): 0
 - Irrigation: Sprinkler
 - Appl. type: AppCrpUsr
 - Texture class: Coarse
 - Eval. depth (cm): 0 to 5
 - OC-Top (%): 5.452
 - Application mode: absolute, relative (selected)
 - 1st application date: 14
 - after: 1st emergenc

At the bottom, there are buttons for "Create PSM-file", "Edit PSM-file", "Mark for batch", "Mark all", "Run Tier 3A", "Evaluation", and "Done".

Tier 3A with PELMO: Parent and metabolites

EFSA Tier 3A

Version
FOCUSPELMO 6.6.1
PELMO Version Number: 5.00

Graph. Output Control
☐ Minimum
☐ Recommended
☒ User Specific

European Scenarios
EFSA
soil
TIER 3

Working examples final

- 09_Maize_2xAppl_Crop_G&M1&M2_G_CTS.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M1_CLC.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M1_CLN.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M1_CLS.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M1_CTC.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M1_CTN.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M1_CTS.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M2_CLC.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M2_CLN.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M2_CLS.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M2_CTC.ptf**
- 09_Maize_2xAppl_Crop_G&M1&M2_M2_CTN.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M2_CTS.ptf
- 11_Maize_1xAppl_SoilSurface_TotalAmountInSoil_A_CLC.ptf
- 11_Maize_1xAppl_SoilSurface_TotalAmountInSoil_A_CLN.ptf
- 11_Maize_1xAppl_SoilSurface_TotalAmountInSoil_A_CLS.ptf
- 11_Maize_1xAppl_SoilSurface_TotalAmountInSoil_A_CTC.ptf
- 11_Maize_1xAppl_SoilSurface_TotalAmountInSoil_A_CTN.ptf
- 11_Maize_1xAppl_SoilSurface_TotalAmountInSoil_A_CTS.ptf

Information obtained from the selected transfer file

Comment: 09_Maize_2xAppl_Crop_GM1M2_M2_CTC.ptf

Compound: M2A (MetaboliteM2) Type of scenario: Total content

DegT50 (d): 250 Crop: Maize

KOC (L/kg): 172.4 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): 8.1 -3.2

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

Incorporation depth (cm): 0 Irrigation: Sprinkler

Appl. type: AppCpUst Texture class: Coarse

Eval. depth (cm): 0 to 5 OC-Top (%): 5.452

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: Parent and metabolites

EFSA Tier 3A

Version
FOCUSPELMO 6.6.1
PELMO Version Number: 5.00

Graph. Output Control
☐ Minimum
☐ Recommended
☒ User Specific

European Scenarios
EFSA
soil
TIER 3

Working examples final

- 09_Maize_2xAppl_Crop_G&M1&M2_G_CTS.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M1_CLC.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M1_CLN.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M1_CLS.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M1_CTC.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M1_CTN.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M1_CTS.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M2_CLC.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M2_CLN.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M2_CLS.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M2_CTC.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M2_CTN.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M2_CTS.ptf
- 11_Maize_1xAppl_SoilSurface_TotalAmountInSoil_A_CLC.ptf
- 11_Maize_1xAppl_SoilSurface_TotalAmountInSoil_A_CLN.ptf
- 11_Maize_1xAppl_SoilSurface_TotalAmountInSoil_A_CLS.ptf
- 11_Maize_1xAppl_SoilSurface_TotalAmountInSoil_A_CTC.ptf
- 11_Maize_1xAppl_SoilSurface_TotalAmountInSoil_A_CTN.ptf
- 11_Maize_1xAppl_SoilSurface_TotalAmountInSoil_A_CTS.ptf

Information obtained from the selected transfer file

Comment: 09_Maize_2xAppl_Crop_GM1M2_M2_CTC.ptf

Compound: M2A (MetaboliteM2) Type of scenario: Total content

DegT50 (d): 250 Crop: Maize

KOC (L/kg): 172.4 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): 8.1 -3.2

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

Incorporation depth (cm): 0 Irrigation: Sprinkler

Appl. type: AppCpUst Texture class: Coarse

Eval. depth (cm): 0 to 5 OC-Top (%): 5.452

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: Parent and metabolites

EFSA Tier 3A

Version
FOCUSPELMO 6.6.1
PELMO Version Number: 5.00

Graph. Output Control
☐ Minimum
☐ Recommended
☒ User Specific

European Scenarios
EFSA
soil
TIER 3

Working examples final

- 09_Maize_2xAppl_Crop_G&M1&M2_G_CTS.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M1_CLC.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M1_CLN.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M1_CLS.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M1_CTC.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M1_CTN.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M1_CTS.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M2_CLC.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M2_CLN.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M2_CLS.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M2_CTC.ptf**
- 09_Maize_2xAppl_Crop_G&M1&M2_M2_CTN.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M2_CTS.ptf
- 11_Maize_1xAppl_SoilSurface_TotalAmountInSoil_A_CLC.ptf
- 11_Maize_1xAppl_SoilSurface_TotalAmountInSoil_A_CLN.ptf
- 11_Maize_1xAppl_SoilSurface_TotalAmountInSoil_A_CLS.ptf
- 11_Maize_1xAppl_SoilSurface_TotalAmountInSoil_A_CTC.ptf
- 11_Maize_1xAppl_SoilSurface_TotalAmountInSoil_A_CTN.ptf
- 11_Maize_1xAppl_SoilSurface_TotalAmountInSoil_A_CTS.ptf

Information obtained from the selected transfer file

Comment: 09_Maize_2xAppl_Crop_GM1M2_M2_CTC.ptf

Compound: M2A (MetaboliteM2) Type of scenario: Total content

DegT50 (d): 250 Crop: Maize

KOC (L/kg): 172.4 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): 8.1 -3.2

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 (%): 5.452

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: Parent and metabolites

EFSA Tier 3A

Version
FOCUSPELMO 6.6.1
PELMO Version Number: 5.00

Graph. Output Control
☐ Minimum
☐ Recommended
☒ User Specific

European Scenarios
EFSA
soil
TIER 3

Working examples final

- 09_Maize_2xAppl_Crop_G&M1&M2_G_CTS.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M1_CLC.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M1_CLN.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M1_CLS.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M1_CTC.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M1_CTN.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M1_CTS.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M2_CLC.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M2_CLN.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M2_CLS.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M2_CTC.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M2_CTN.ptf
- 09_Maize_2xAppl_Crop_G&M1&M2_M2_CTS.ptf
- 11_Maize_1xAppl_SoilSurface_TotalAmountInSoil_A_CLC.ptf
- 11_Maize_1xAppl_SoilSurface_TotalAmountInSoil_A_CLN.ptf
- 11_Maize_1xAppl_SoilSurface_TotalAmountInSoil_A_CLS.ptf
- 11_Maize_1xAppl_SoilSurface_TotalAmountInSoil_A_CTC.ptf
- 11_Maize_1xAppl_SoilSurface_TotalAmountInSoil_A_CTN.ptf
- 11_Maize_1xAppl_SoilSurface_TotalAmountInSoil_A_CTS.ptf

Information obtained from the selected transfer file

Comment: 09_Maize_2xAppl_Crop_GM1M2_M2_CTC.ptf

Compound: M2A (MetaboliteM2) Type of scenario: Total content

DegT50 (d): 250 Crop: Maize

KOC (L/kg): 172.4 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): 8.1 -3.2

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

Incorporation depth (cm): 0 Irrigation: Sprinkler

Appl. type: AppCpUst Texture class: Coarse

Eval. depth (cm): 0 to 5 OC-Top (%): 5.452

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: 09_Maize_2xAppl_Crop_G&M1&M2_M2_CTC

Crop: Maize ERD (cm): 5

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

Temp shift (°C): -3.200 Rain factor: 1.000 OC (%): 5.45

Show tabular output

Echo **PEC soil** Mass Balance Summary

Create Diagrams (Daily Time Step)

Total content in soil at 1 cm for Metabolite A2

☐ Cumulative from: January 33

☒ Non-cumulative to: December 52

Show Diagram

Done

PECs in soil for Central Europe following spray application of compound G
Substance of concern: M2

Table of actual and time weighted average concentrations in soil

Tier 3A simulation:

*** FOCUS PELMO 6. 6. 1 *** (PELMO 5.0)
 Compound: 09_Maize_2xAppl_Crop_G:M1:M2_M2_CTC
 Soil: Coarse (5.45% 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: M2A (Metabolite)

TWA(d)	PEC(mg/kg)	Begin TWA(d)
0	0.2034560	31 March 48
1	0.2034560	31 March 48
2	0.2032790	31 March 48
3	0.2026453	31 March 48
4	0.2023200	31 March 48
7	0.2019243	31 March 48
14	0.2017041	31 March 48
21	0.2009212	31 March 48
28	0.2004446	31 March 48
56	0.1967837	31 March 48
100	0.1826482	31 March 48
Plateau (20 cm)	0.2048475	29 May 48
Conc. after 90 d	0.1993714	27 August 50
Conc. after 120 d	0.1971600	26 September 50
Conc. after 165 d	0.1965097	10 November 50
Conc. after 200 d	0.1941310	15 December 50
Conc. after 270 d	0.1901215	23 February 51
Conc. after 320 d	0.1904435	14 April 51
Conc. after 365 d	0.1958610	29 May 51

Buttons: Copy, Print, Done

Tier	PECmax (TWA=0)
1 (PERSAM)	4.68
2 (PERSAM)	2.42
3 (PELMO)	0.20



Subscribe to

www.efsa.europa.eu/en/news/newsletters
www.efsa.europa.eu/en/rss



Engage with careers

www.efsa.europa.eu/en/engage/careers



Follow us on Twitter

@efsa_eu
@plants_efsa
@methods_efsa