June 4-5th 2019

PERSAM Worked-examples: Application by soil incorporation

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EFSA Trainees

Trusted science for safe food

efsa
European Food Safety Authority

Example 4 (annual crops, soil incorporation)

1) Evenly distributed incorporation of granules over a certain soil depth

2) Placing of granules at a certain soil depth

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

Evenly distributed incorporation of granules over a certain soil depth

Crop:
Maize

Number of applications:
1 application (1 kg/ha)

Type of application:
Granules evenly incorporated (mixed) over a soil depth (z_{inc}) of 10 cm

Time of application:
2 weeks before planting of maize (30 days before emergence)

Substance properties:
DegT50 (*geomean*): 250 days
Kom (*geomean*): 1000 (L/kg)
Molar mass: 300 g/mol
Water solubility: 0.1 mg/L

Substance property	Unit	A
Molar mass	(g/mol)	300
Water solubility (20°C)	(mg/L)	0.1
Vapour pressure (20°C)	(Pa)	10^{-8}
DegT50[(a)] (geomean)	(days)	250
Molar activation energy	(kJ/ mol^{-1})	65.4
Exponent for the effect of liquid	(–)	0.7
K_{om} (geomean)	(L/kg)	1,000
K_{om} in dry soil[(e)]	(L/kg)	10^5
$1/n$	(–)	0.9
DegT50 on crop surface	[(d)]	10
Wash-off factor[(g)]	(mm^{-1})	0.1
Plant uptake factor	(–)	0
Molar formation fraction (arithmetic mean)	(–)	–

Evenly distributed incorporation of granules over a certain soil depth

PERSAM Graphical shell

Create a new project

PERSAM

v 3.0.0-SNAPSHOT

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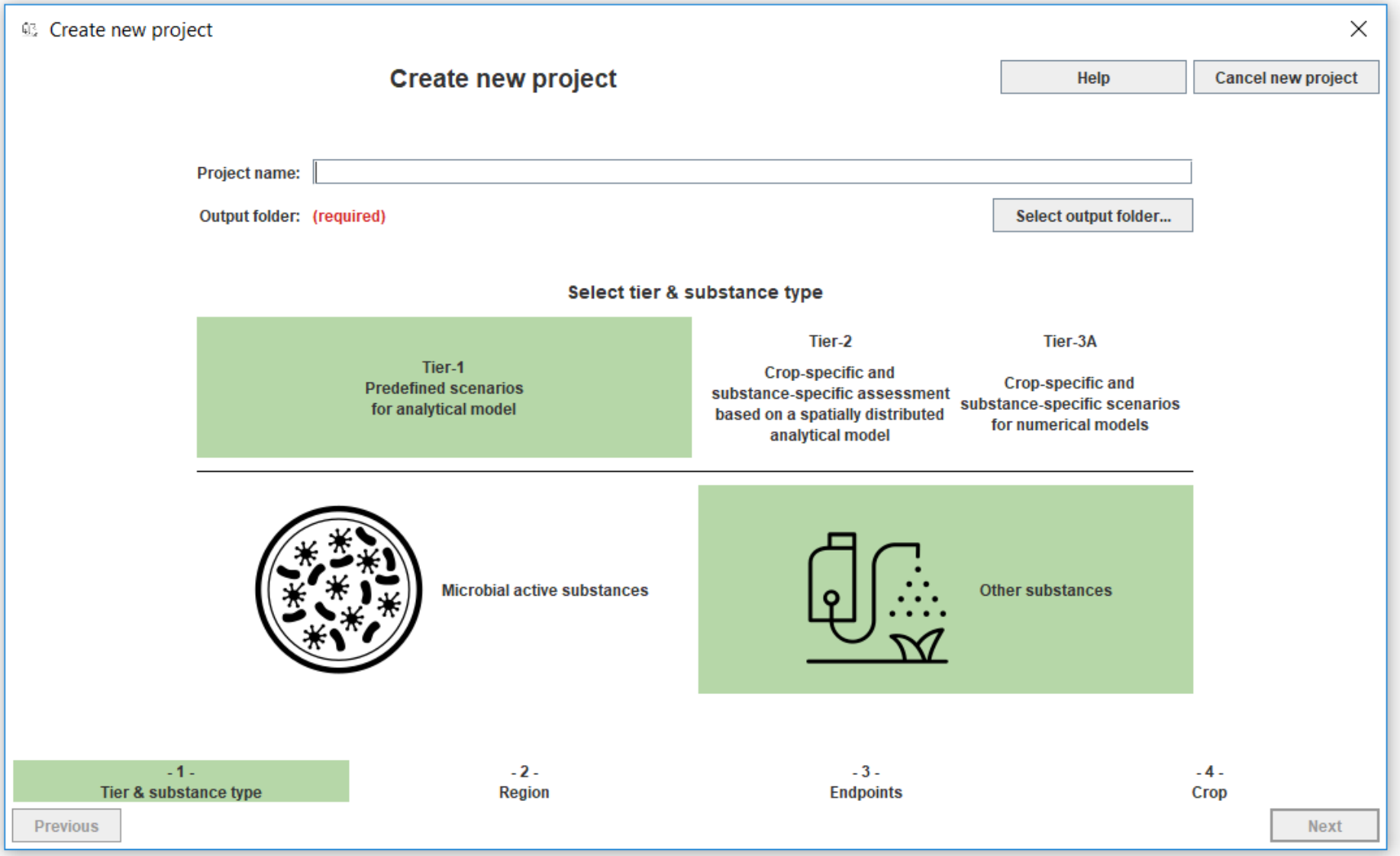
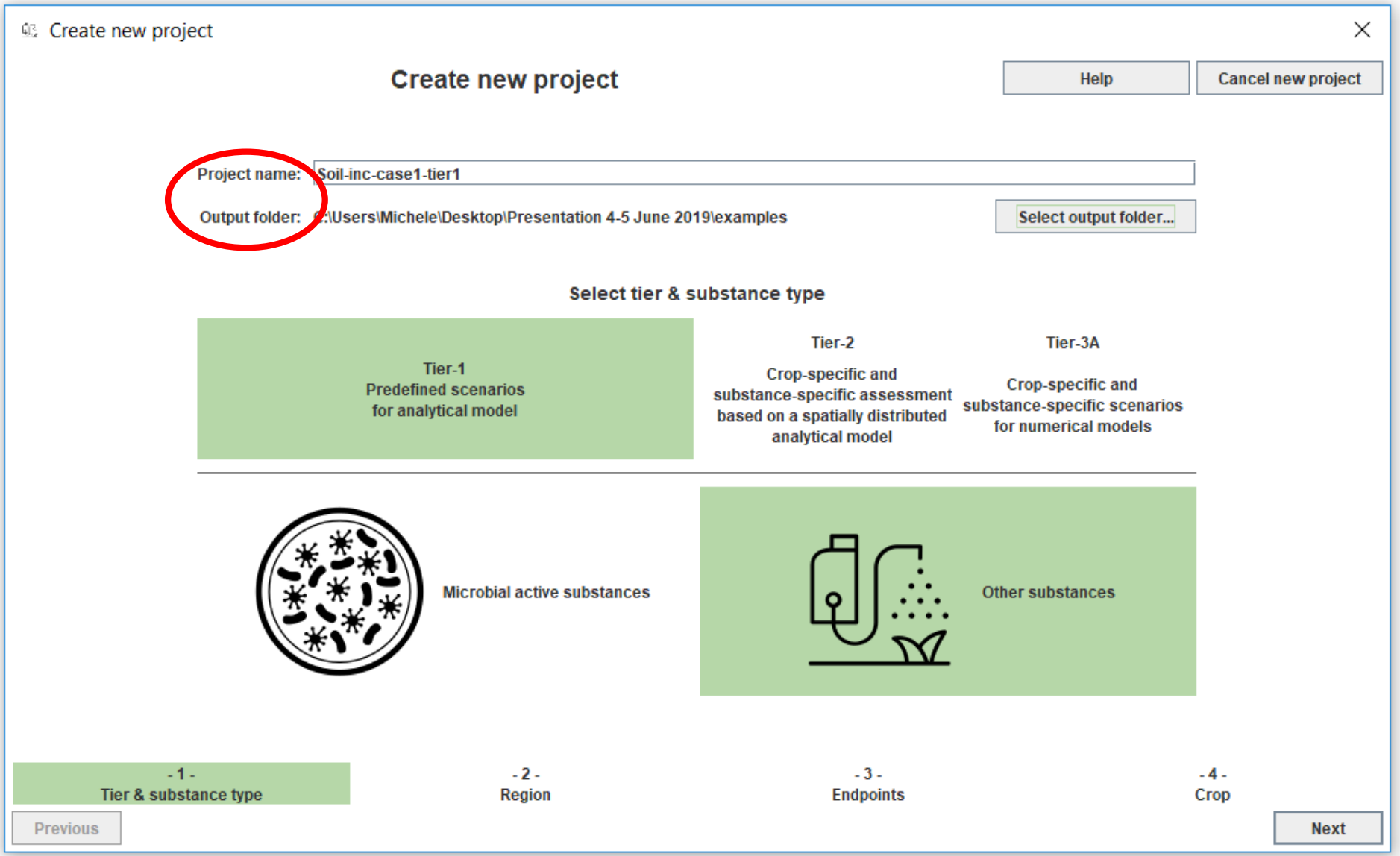
at the request of EFSA http://www.efsa.eu

Evenly distributed incorporation of granules over a certain soil depth

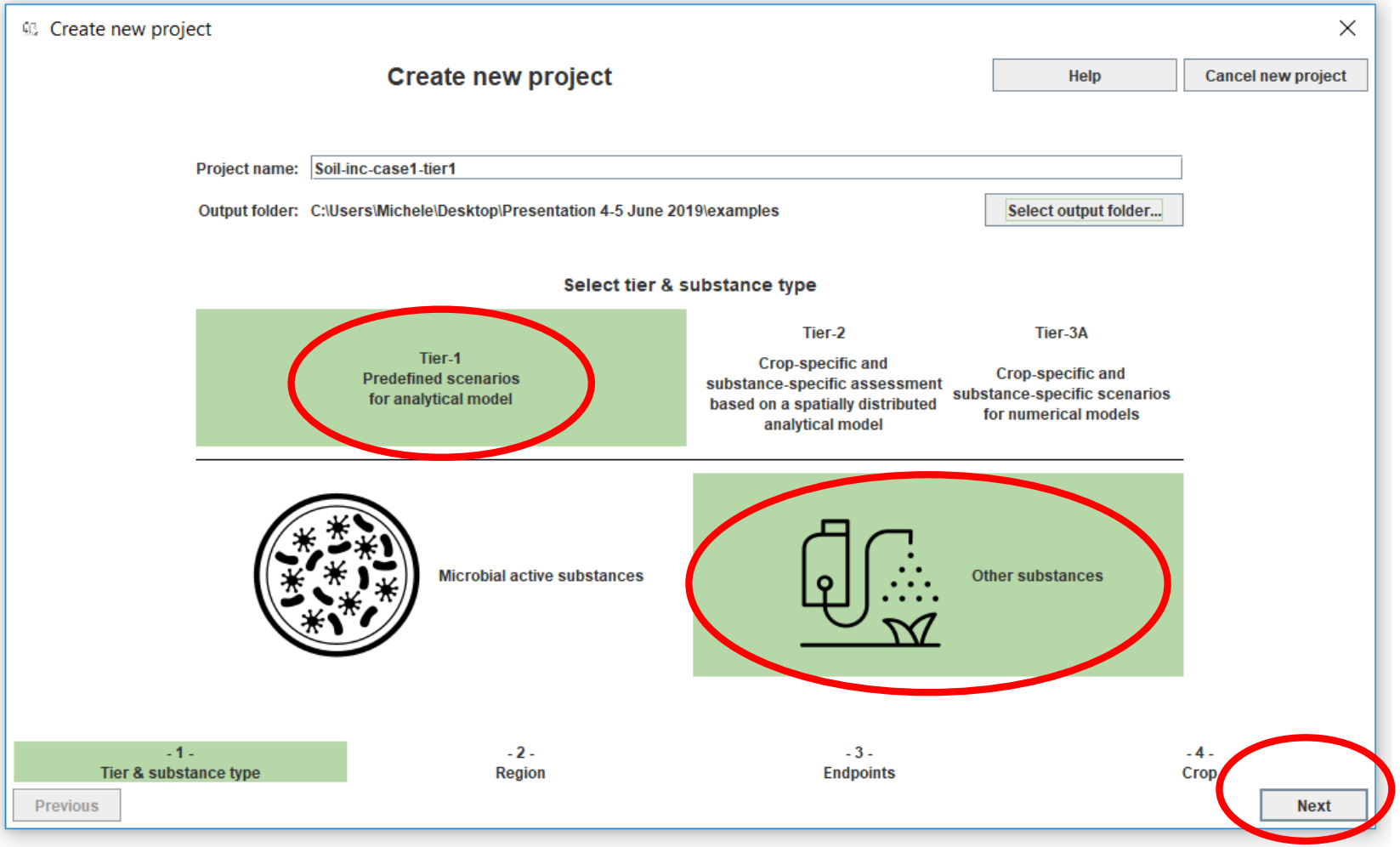


Evenly distributed incorporation of granules over a certain soil depth



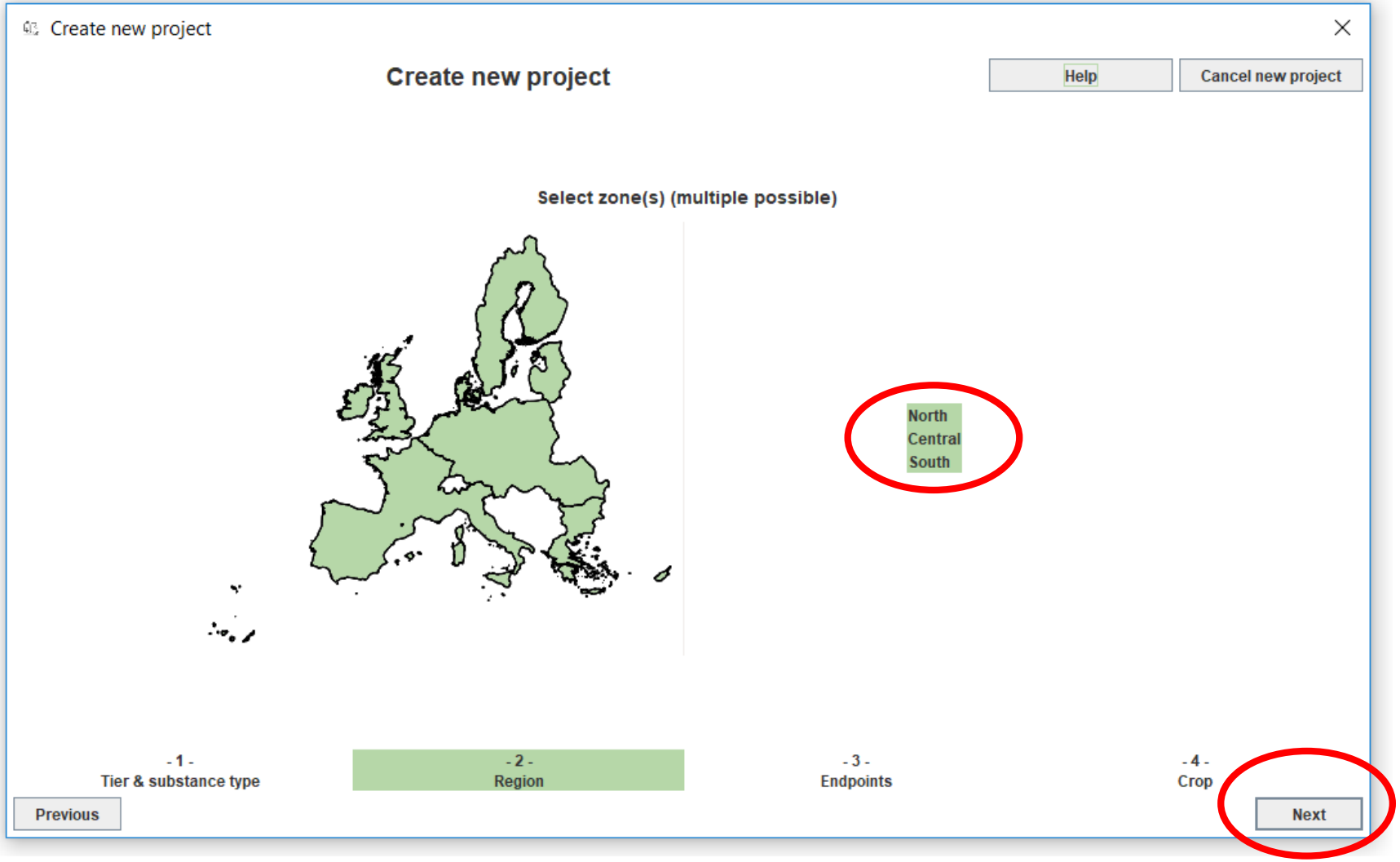
Tier 1. Evenly distributed incorporation of granules over a certain soil depth

At **Tier 1** soil incorporation is not taken into account
Same assumptions for Example 1 and 2



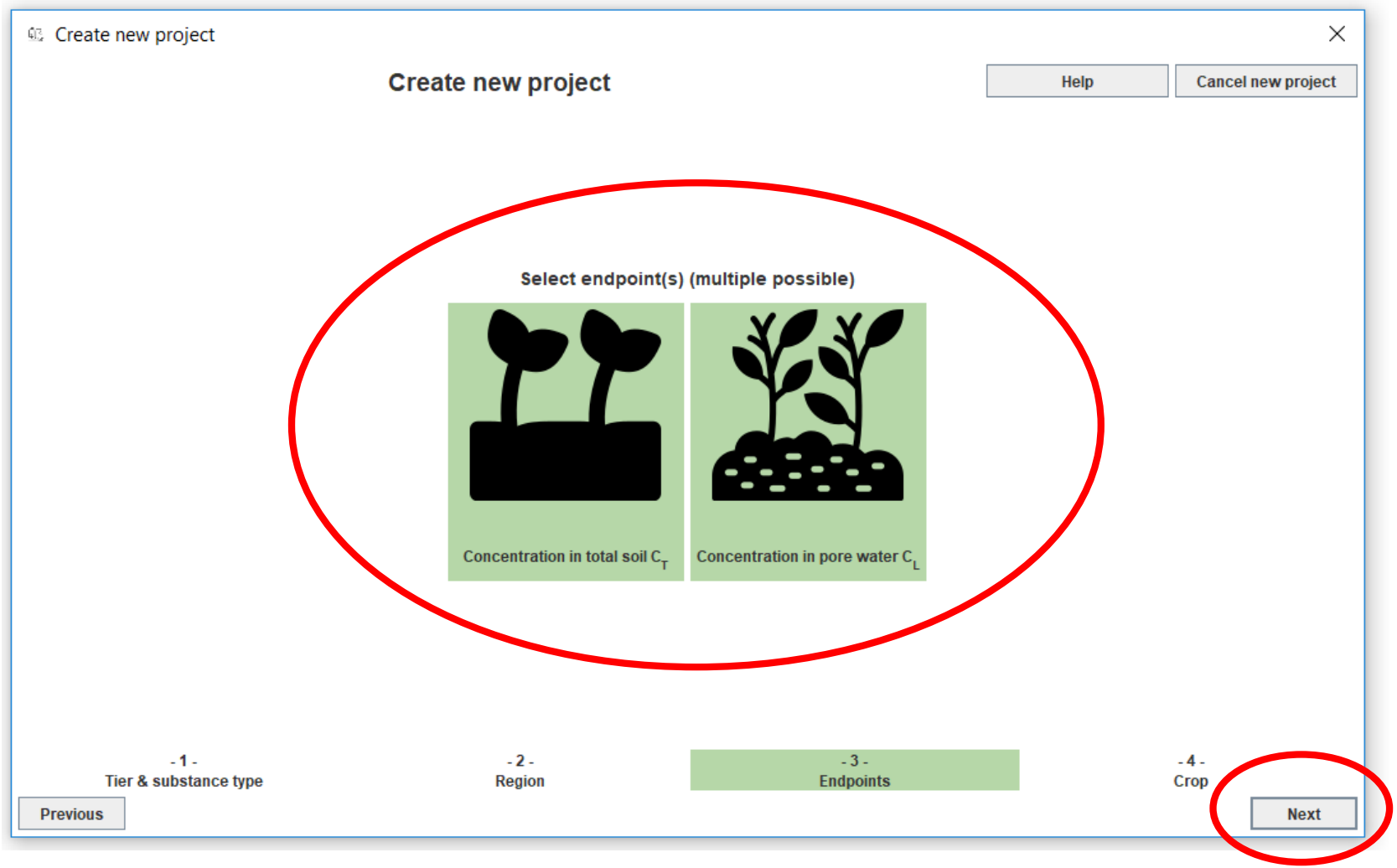
Tier 1. Evenly distributed incorporation of granules over a certain soil depth

Regulatory zones



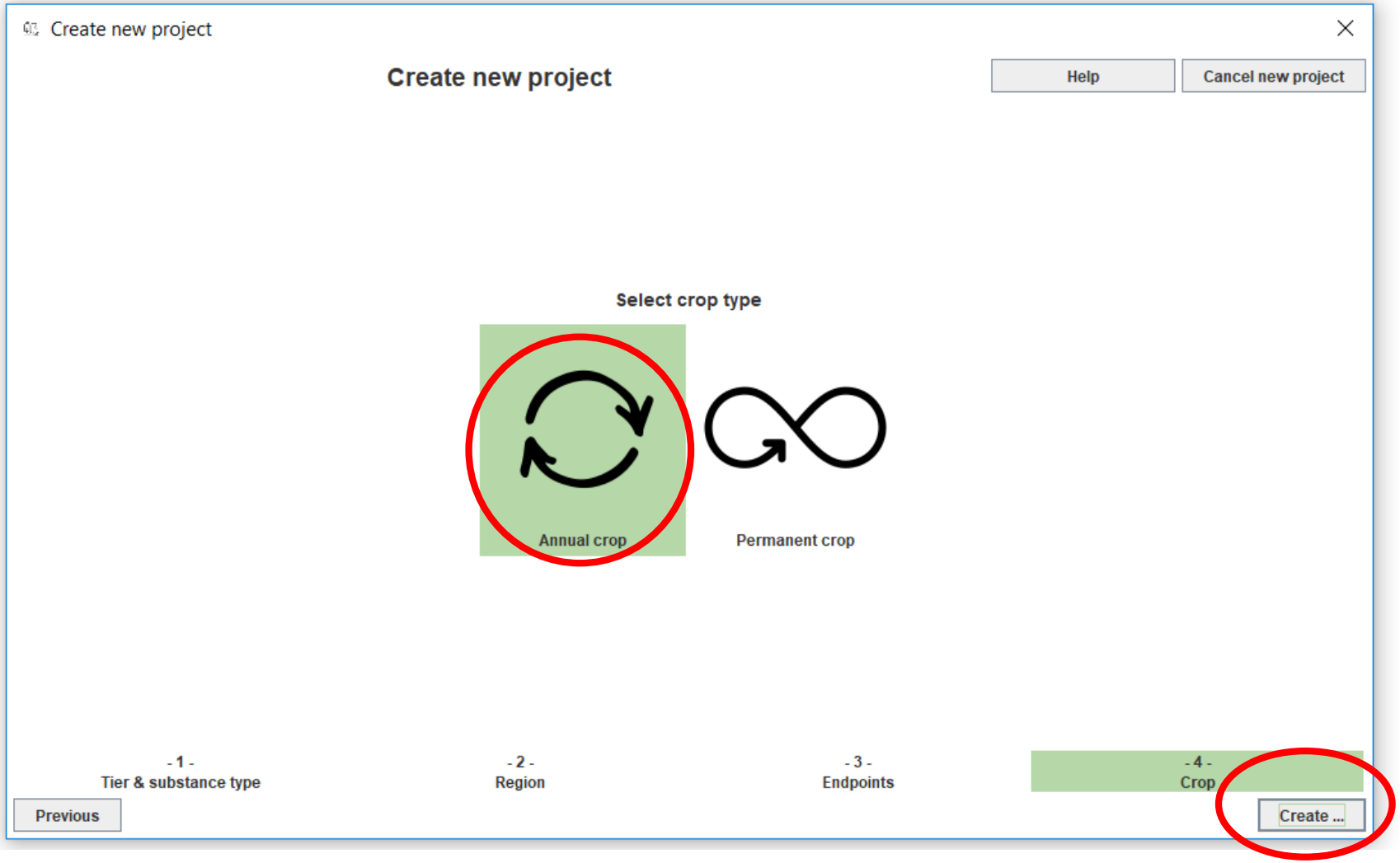
Tier 1. Evenly distributed incorporation of granules over a certain soil depth

PECs selection



Tier 1. Evenly distributed incorporation of granules over a certain soil depth

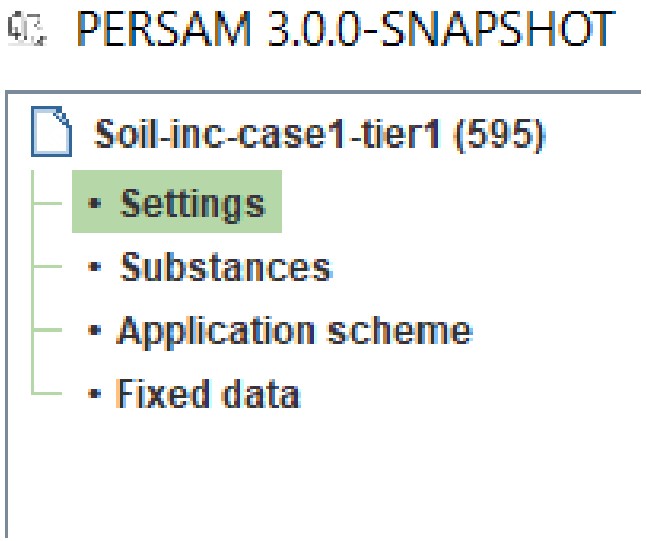
Crop type selection: at **Tier 1** only 2 options available

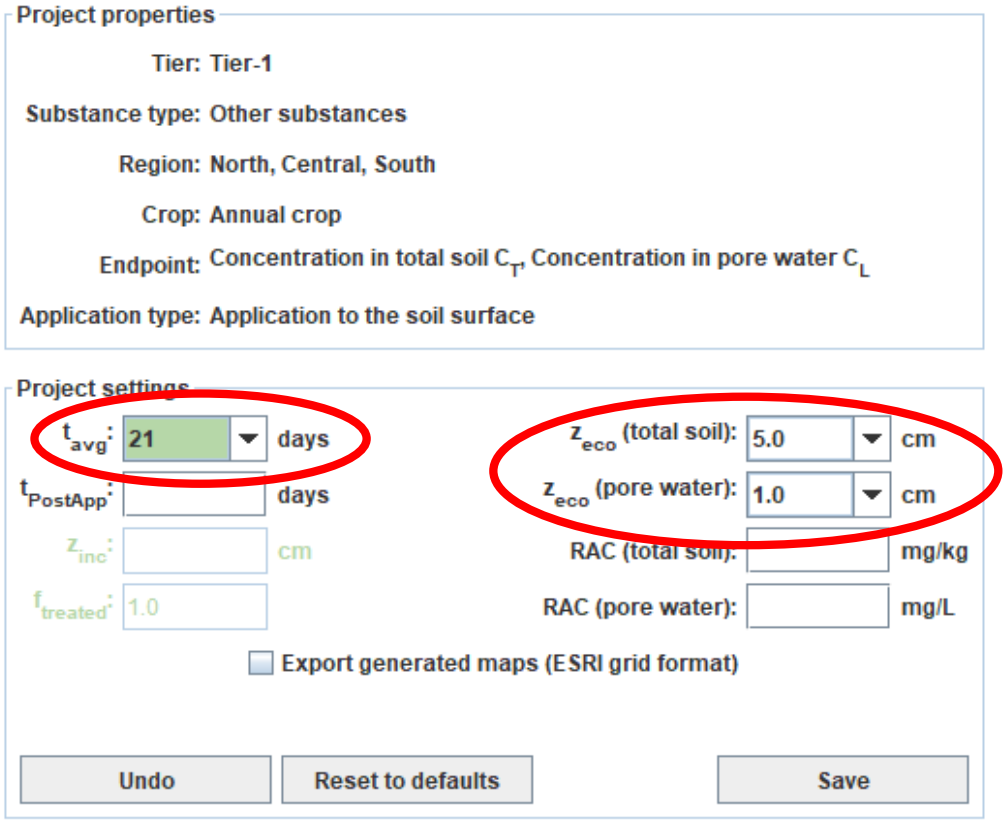


Tier 1. Evenly distributed incorporation of granules over a certain soil depth

Scenario parameterisation

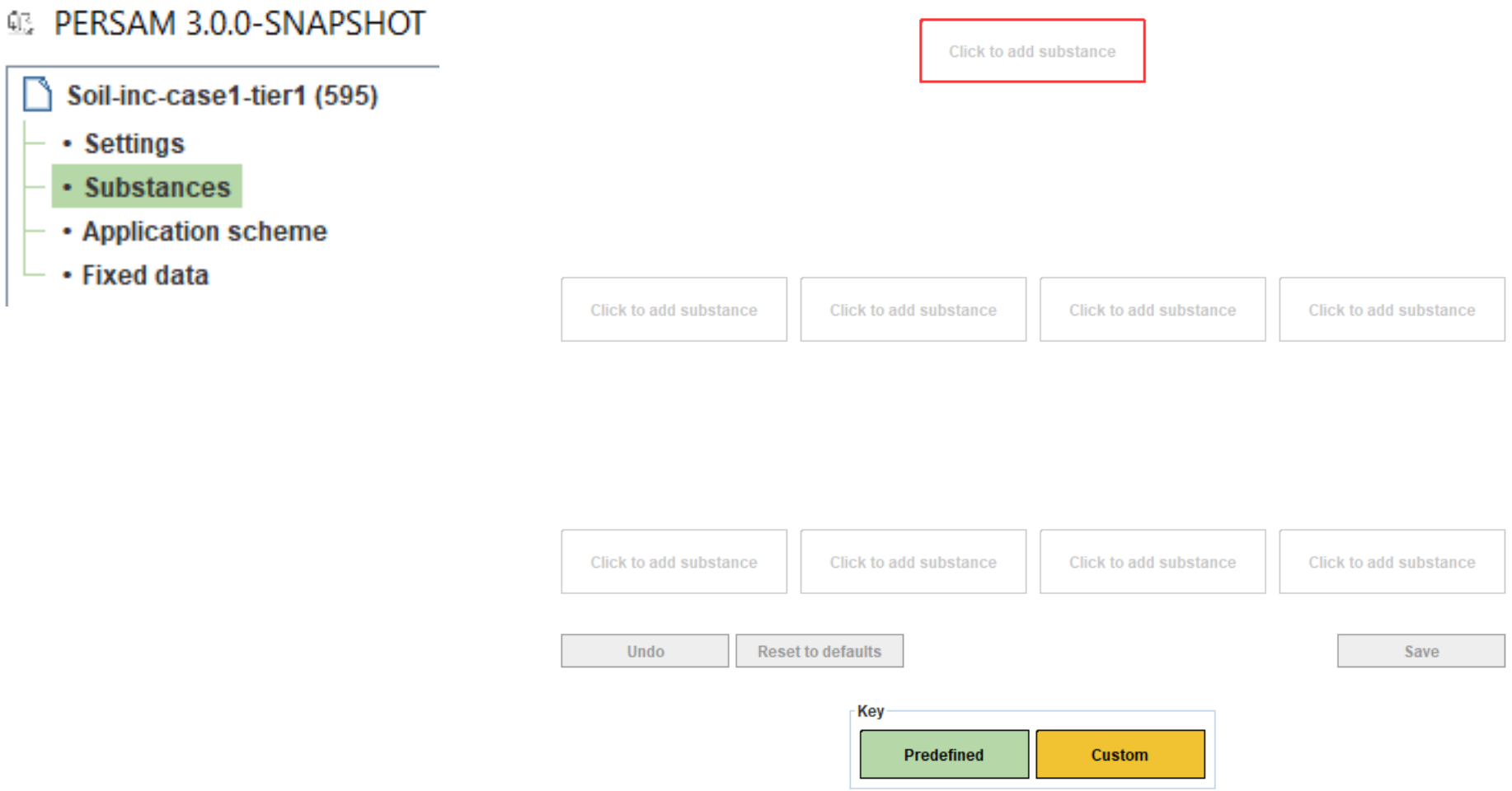
Ecotoxicological averaging depth in soil and pore water **(z_{eco})**
Time weighted average **(t_{avg})**





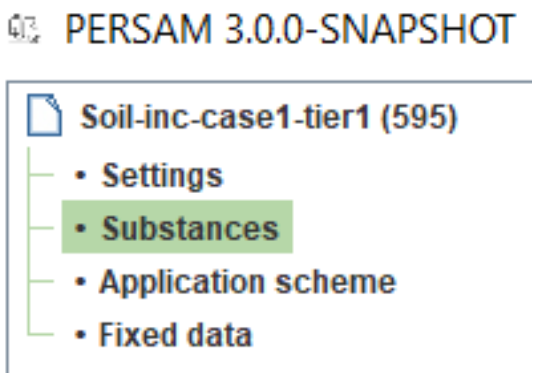
Tier 1. Evenly distributed incorporation of granules over a certain soil depth

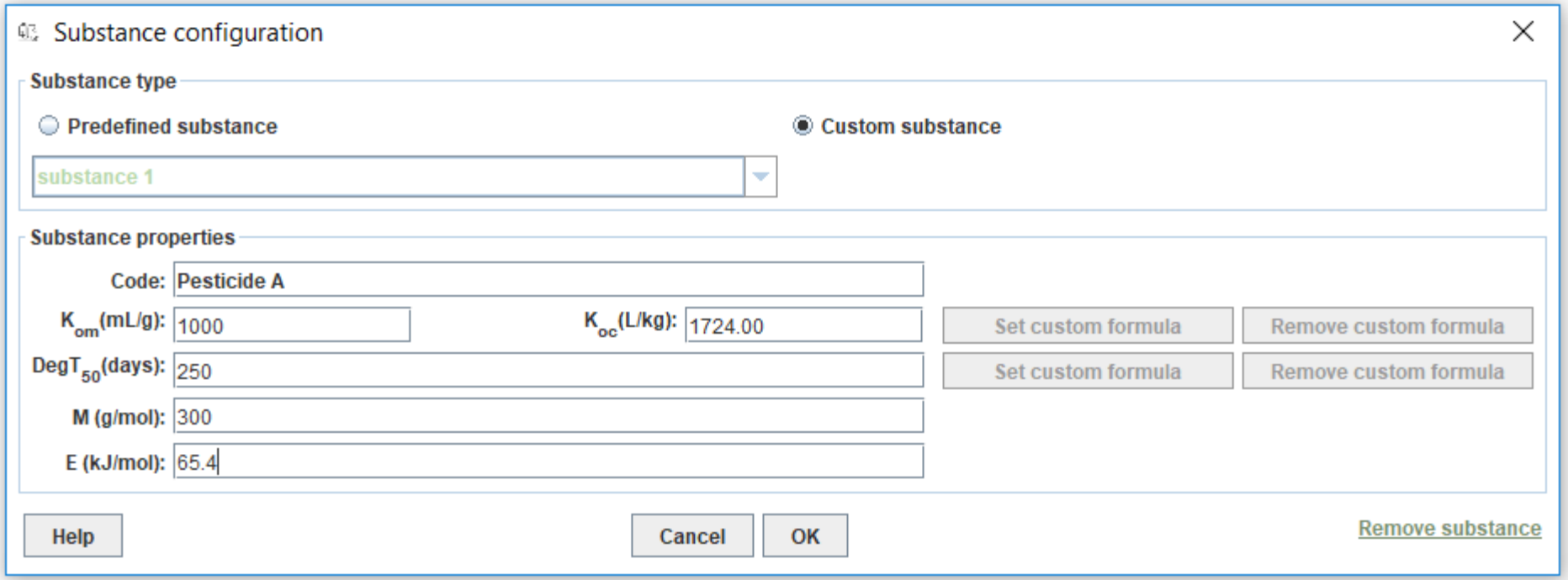
Pesticide input parameters



Tier 1. Evenly distributed incorporation of granules over a certain soil depth

Pesticide input parameters

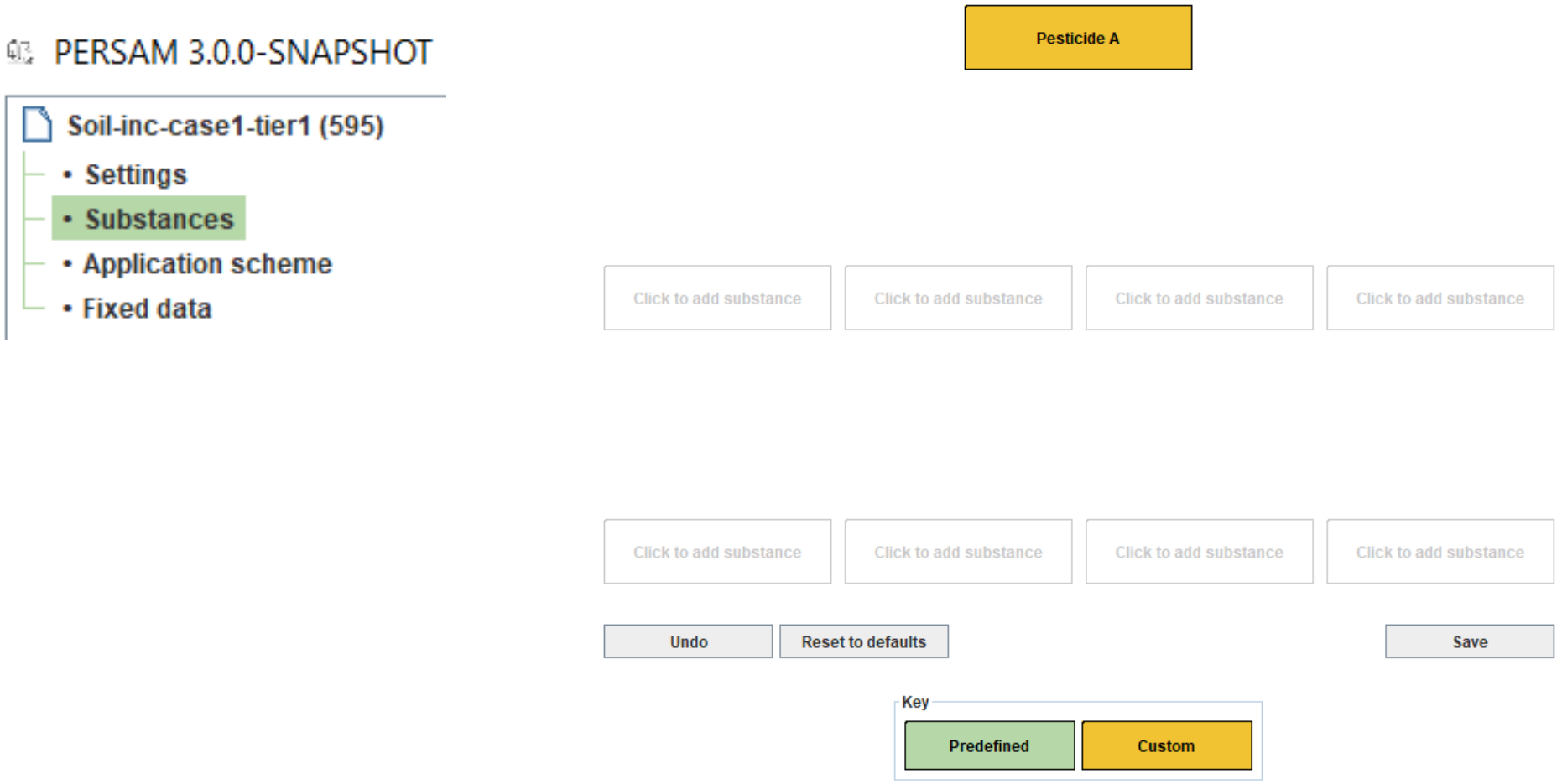




Tier 1. Evenly distributed incorporation of granules over a certain soil depth

Pesticide input parameters

Degradation pathway (no metabolites considered)

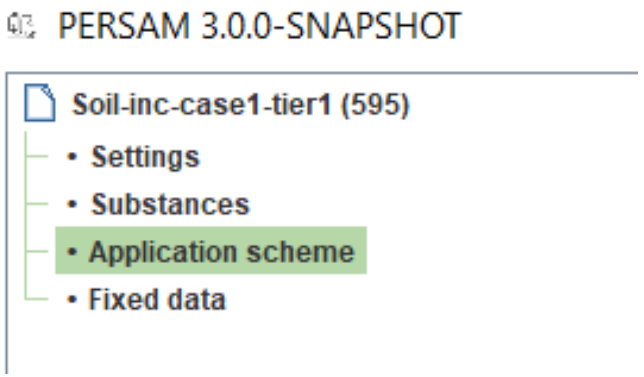


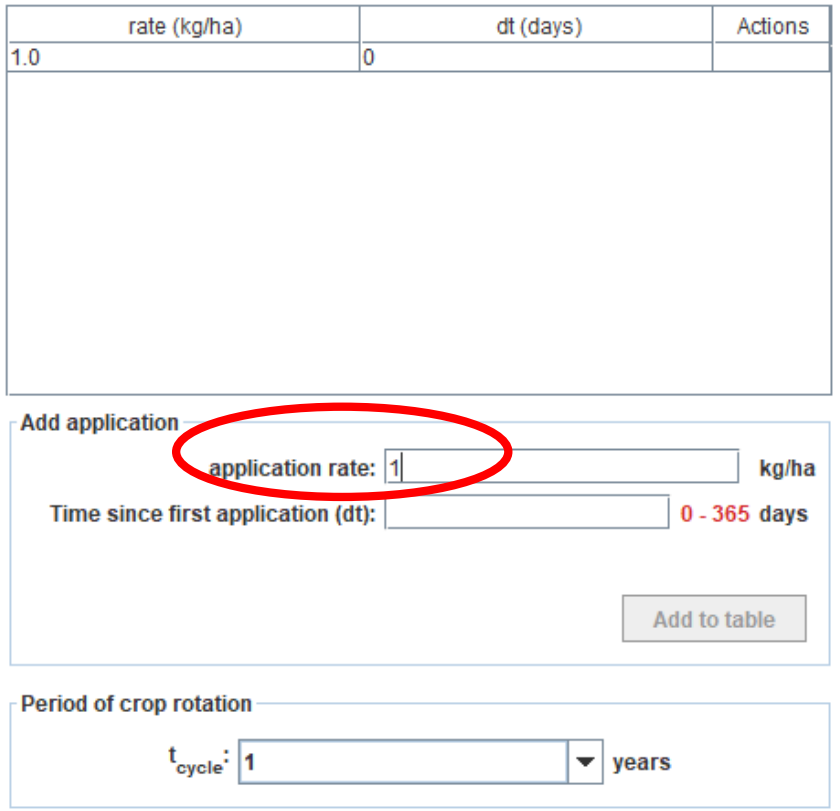
Tier 1. Evenly distributed incorporation of granules over a certain soil depth

Application scheme

Single application

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

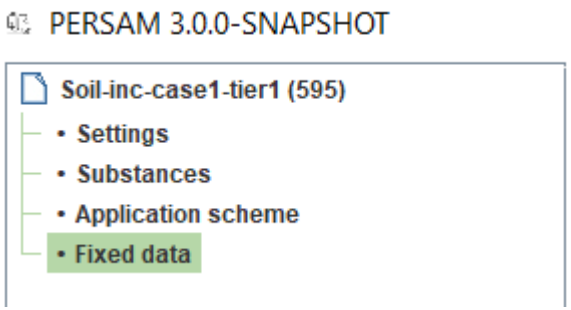




Tier 1. Evenly distributed incorporation of granules over a certain soil depth

Fixed parameters

1 value (average) for each regulatory zone is considered at **Tier 1**



Concentration in total soil

Zone	T_{arit}(°C)	T_{arr}(°C)	θ_{fc}(m^3/m^3)	ρ(kg/L)	f_{om}(kg/kg)
North	5.7	7.6	0.244	0.707	0.22
Central	7.4	9.3	0.244	0.934	0.122
South	10.2	11.7	0.349	1.117	0.07

Concentration in pore water

Zone	T_{arit}(°C)	T_{arr}(°C)	θ_{fc}(m^3/m^3)	ρ(kg/L)	f_{om}(kg/kg)
North	8.0	9.2	0.349	1.371	0.025
Central	9.3	11.3	0.349	1.432	0.018
South	15.4	16.7	0.349	1.521	0.01

Constants

Adjustment factor	Total soil	Pore water	R (kJ/mol/K)	T_{ref}(°C)
scenario	1.4	1.6	0.008314	20.0
model	3.0	4.0		

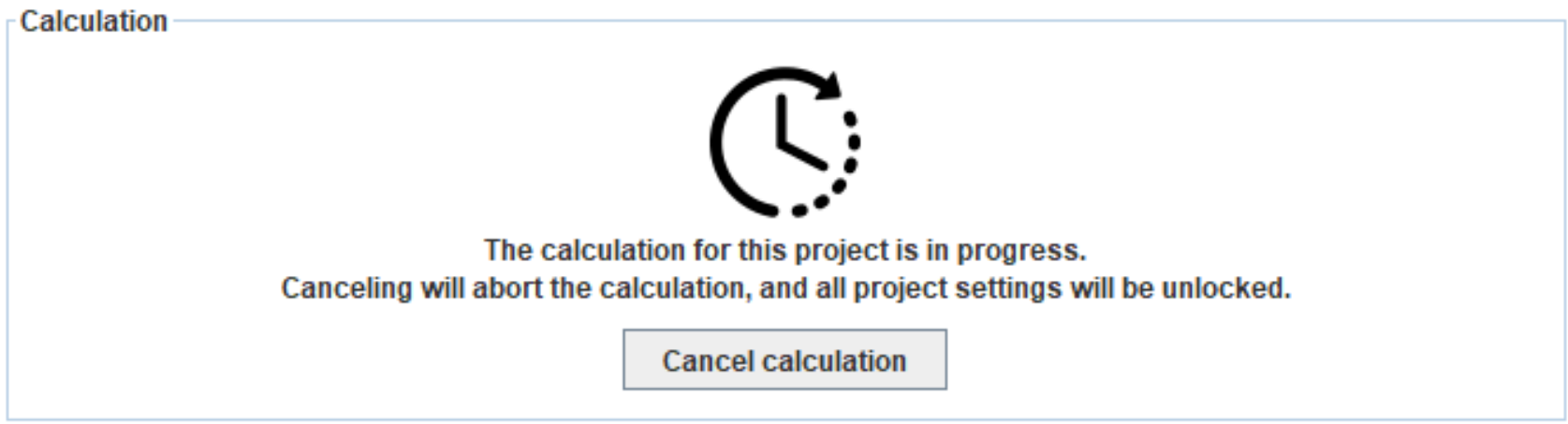
Not all fixed values are relevant at all tiers and for microbial calculations.
More info see user manual.

Calculation

The calculation for this project has not started yet.
As soon as you start the calculation, all project settings will be locked.

Start calculation

Tier 1. Evenly distributed incorporation of granules over a certain soil depth

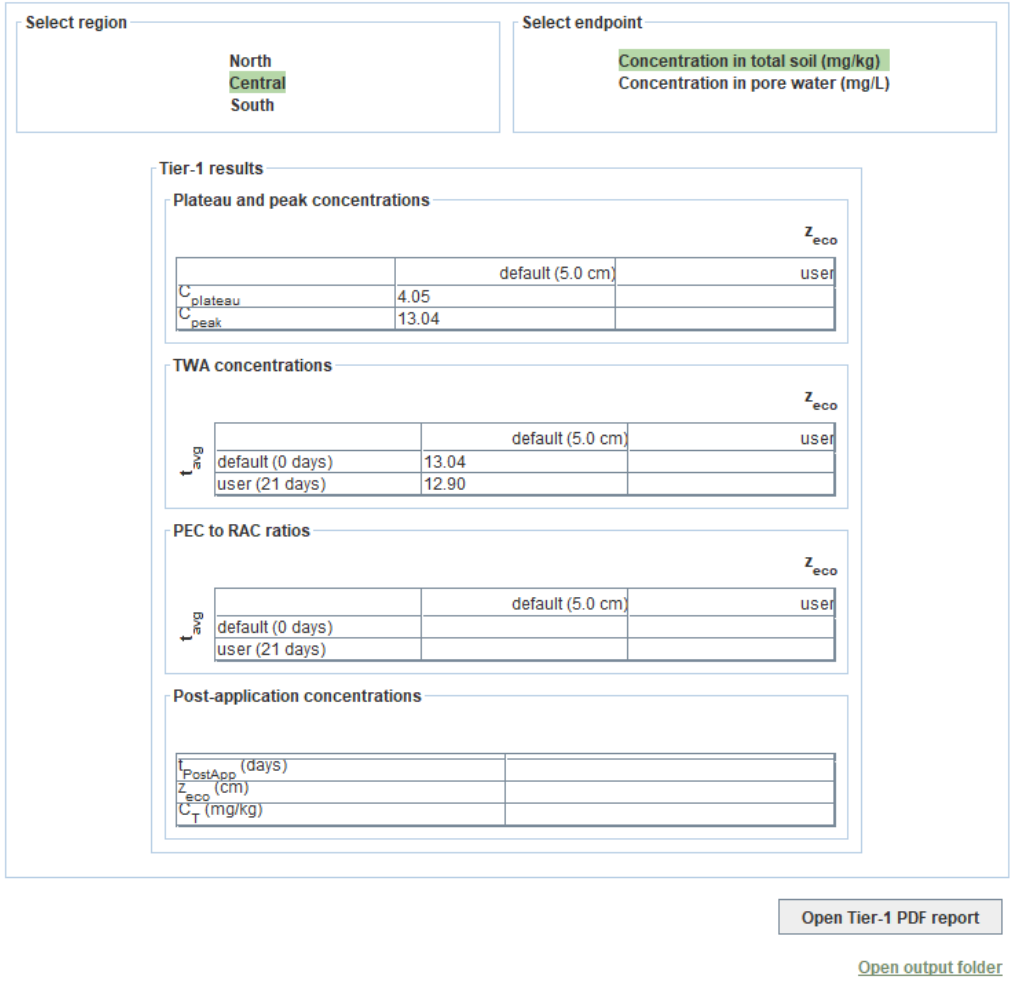


Tier 1. Evenly distributed incorporation of granules over a certain soil depth

Model output

Results of **Tier 1**

Export results in pdf/word format



Select region

North
Central
South

Select endpoint

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

Tier-1 results

Plateau and peak concentrations

z_{eco}

	default (5.0 cm)	user
$C_{plateau}$	4.05	
C_{peak}	13.04	

TWA concentrations

z_{eco}

t_{avg}	default (5.0 cm)	user
default (0 days)	13.04	
user (21 days)	12.90	

PEC to RAC ratios

z_{eco}

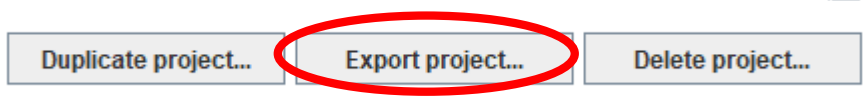
t_{avg}	default (5.0 cm)	user
default (0 days)		
user (21 days)		

Post-application concentrations

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

Open Tier-1 PDF report

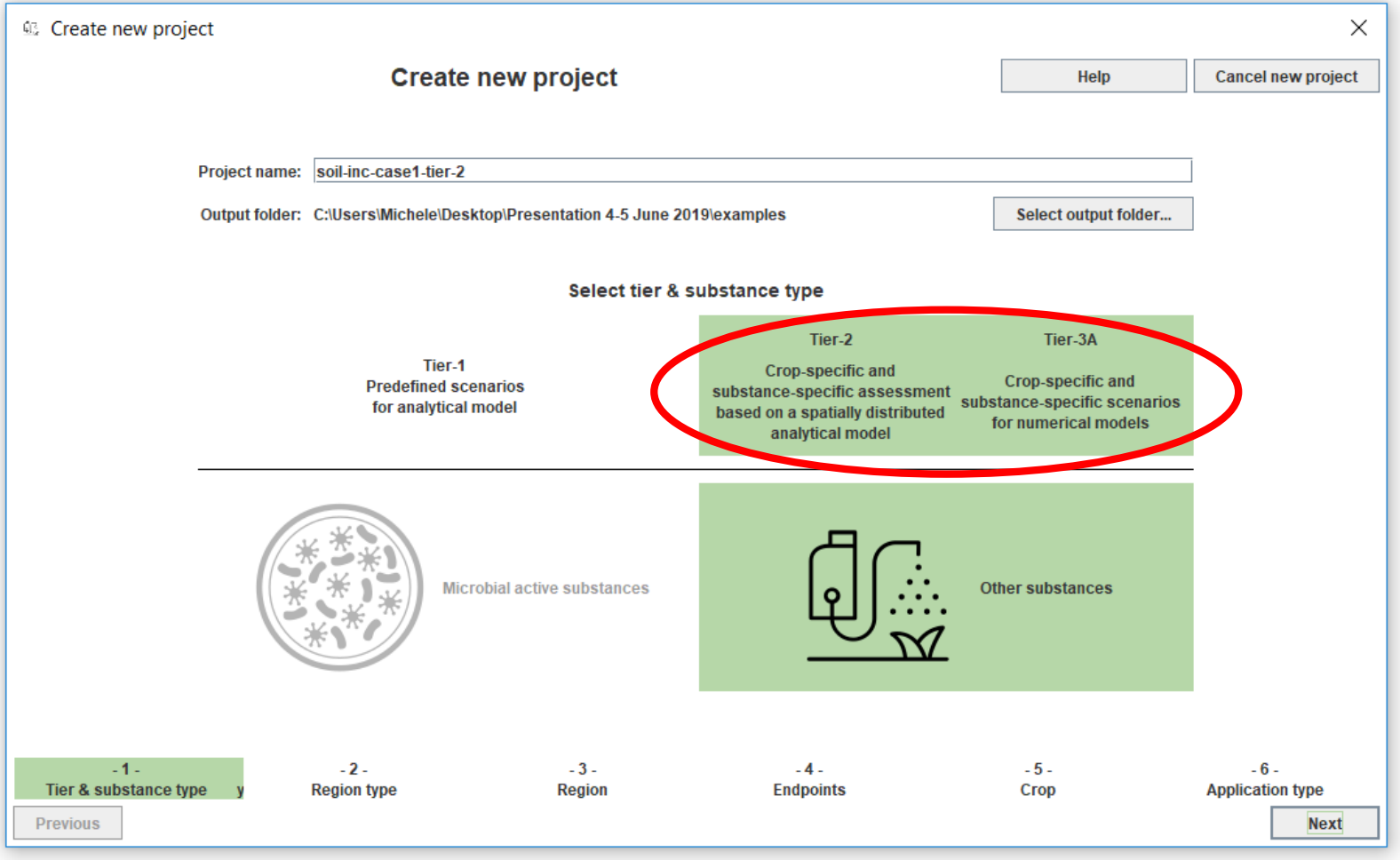
Open output folder



Duplicate project... Export project... Delete project...

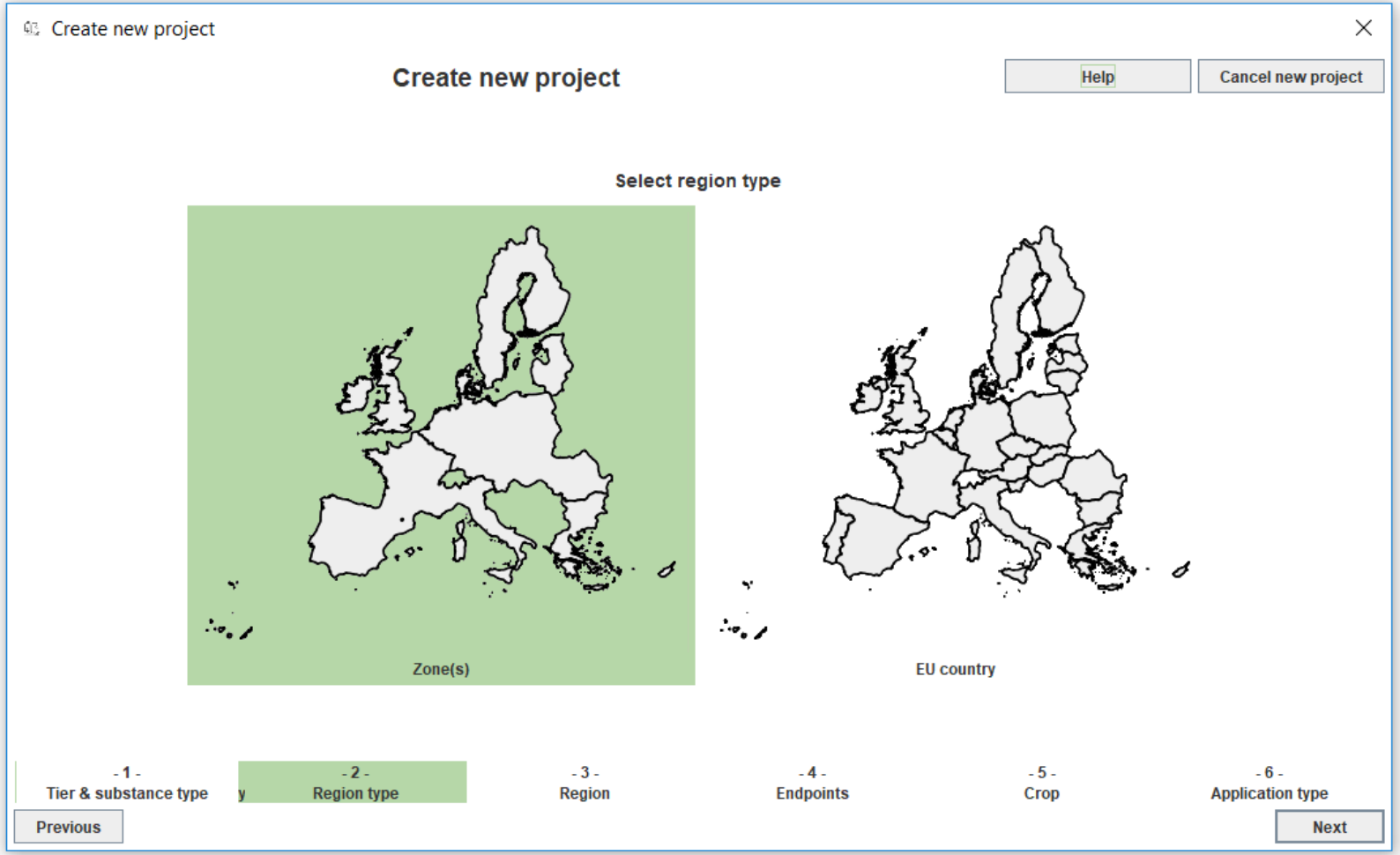
Tier 2. Evenly distributed incorporation of granules over a certain soil depth

Scenario parameterisation at **Tier 2** and **Tier 3A** is unified whilst creating the PERSAM transfer file for higher tier assessment

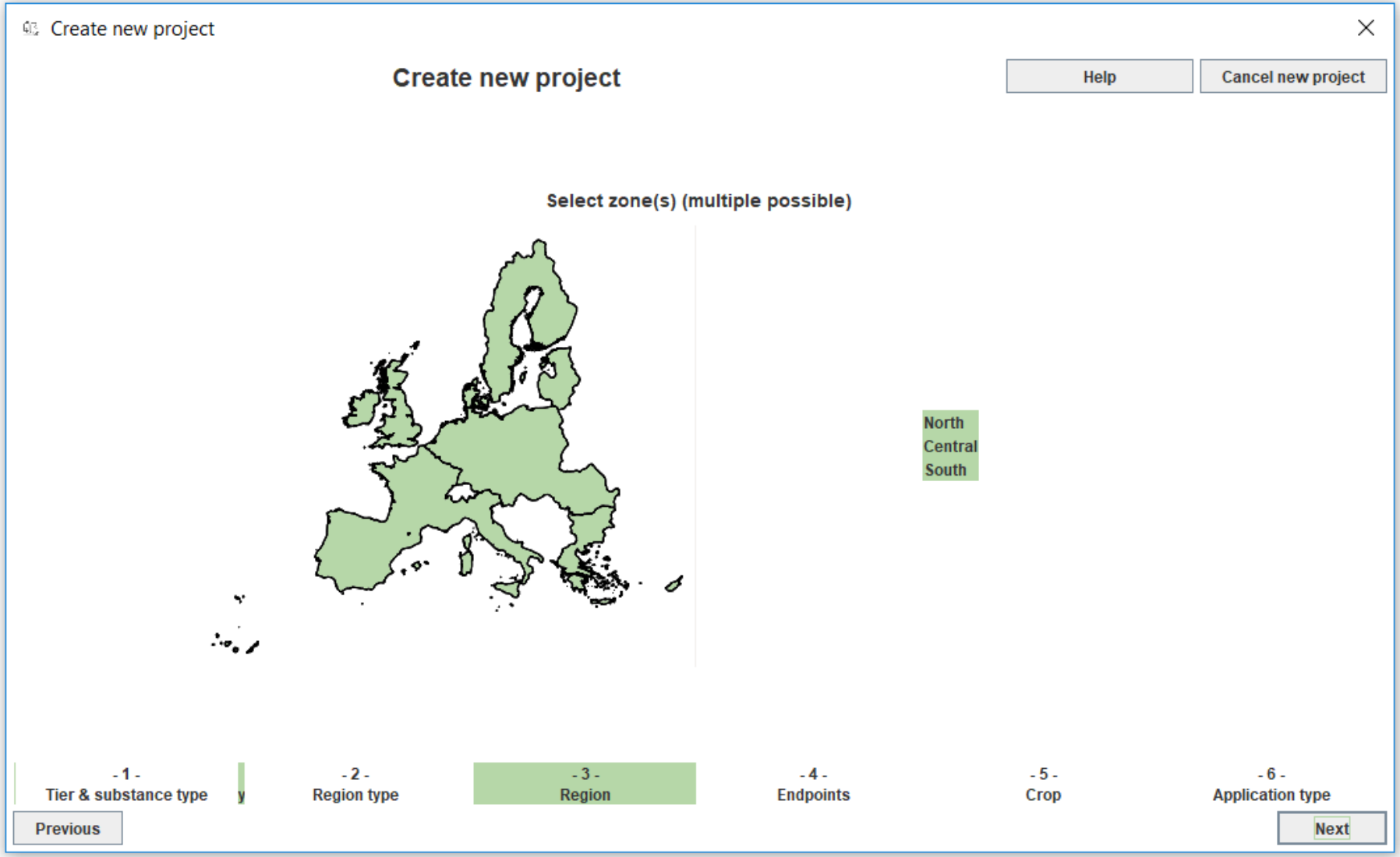


Tier 2. Evenly distributed incorporation of granules over a certain soil depth

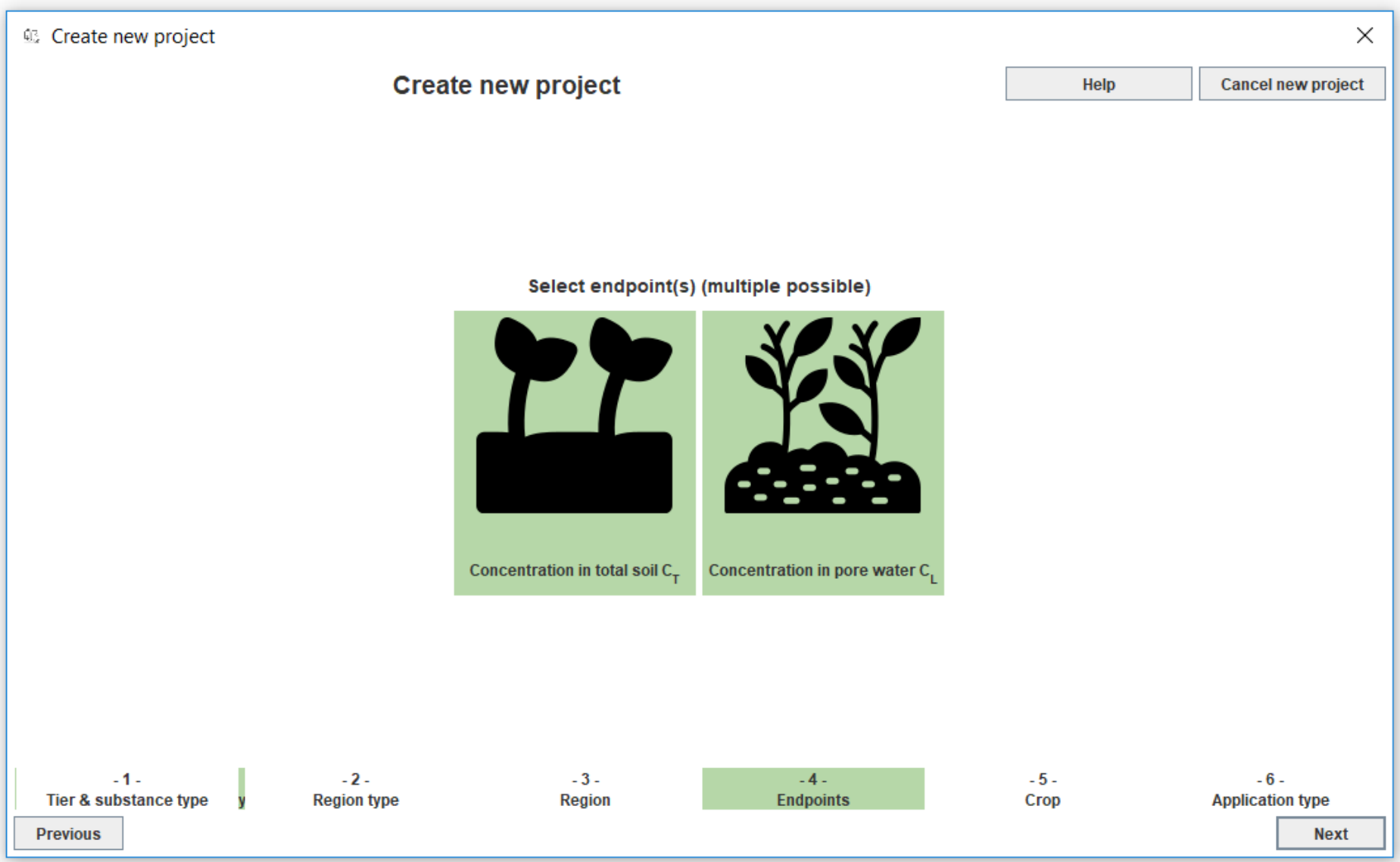
Single EU Countries are available for modelling at **Tier 2**



Tier 2. Evenly distributed incorporation of granules over a certain soil depth

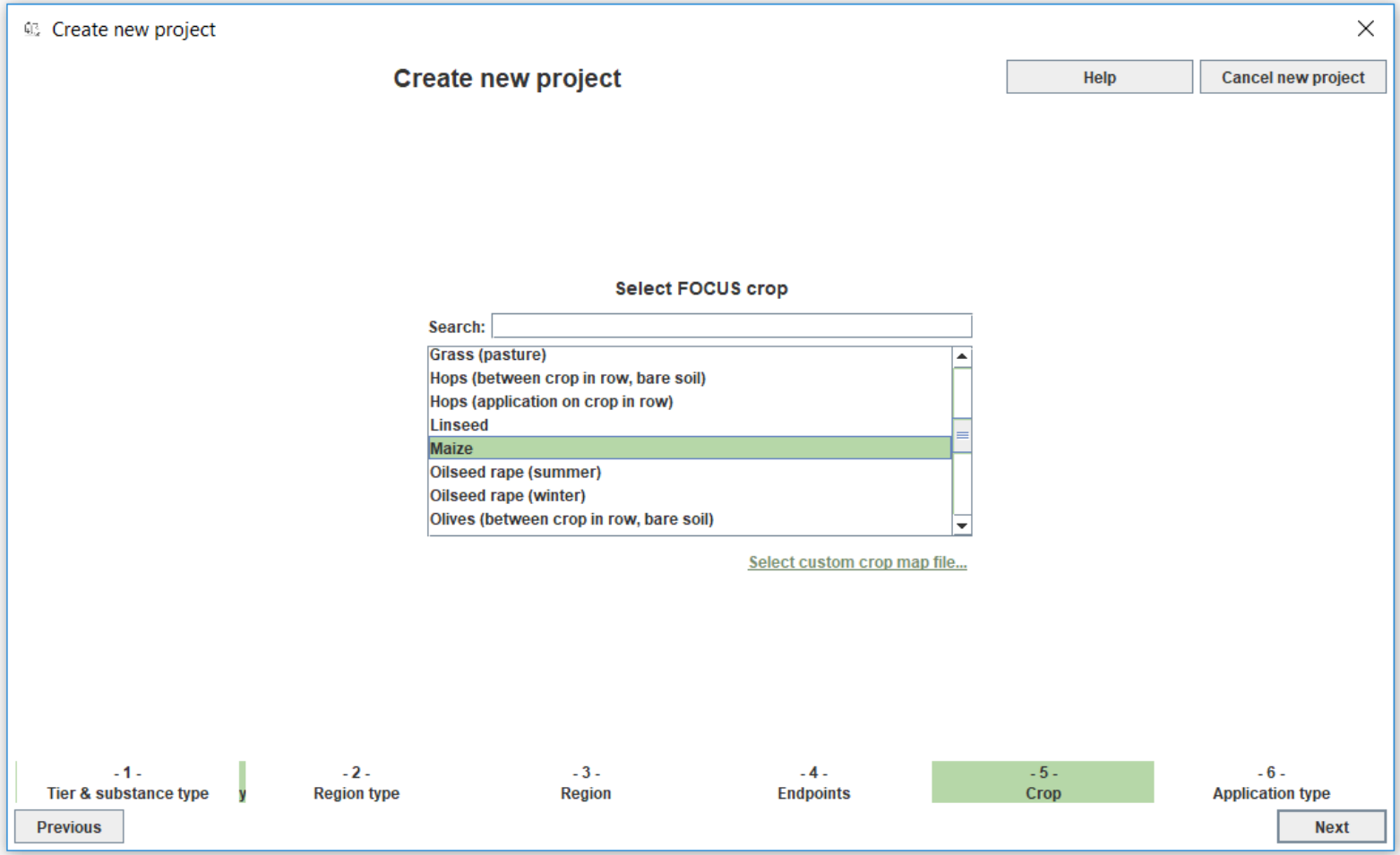


Tier 2. Evenly distributed incorporation of granules over a certain soil depth



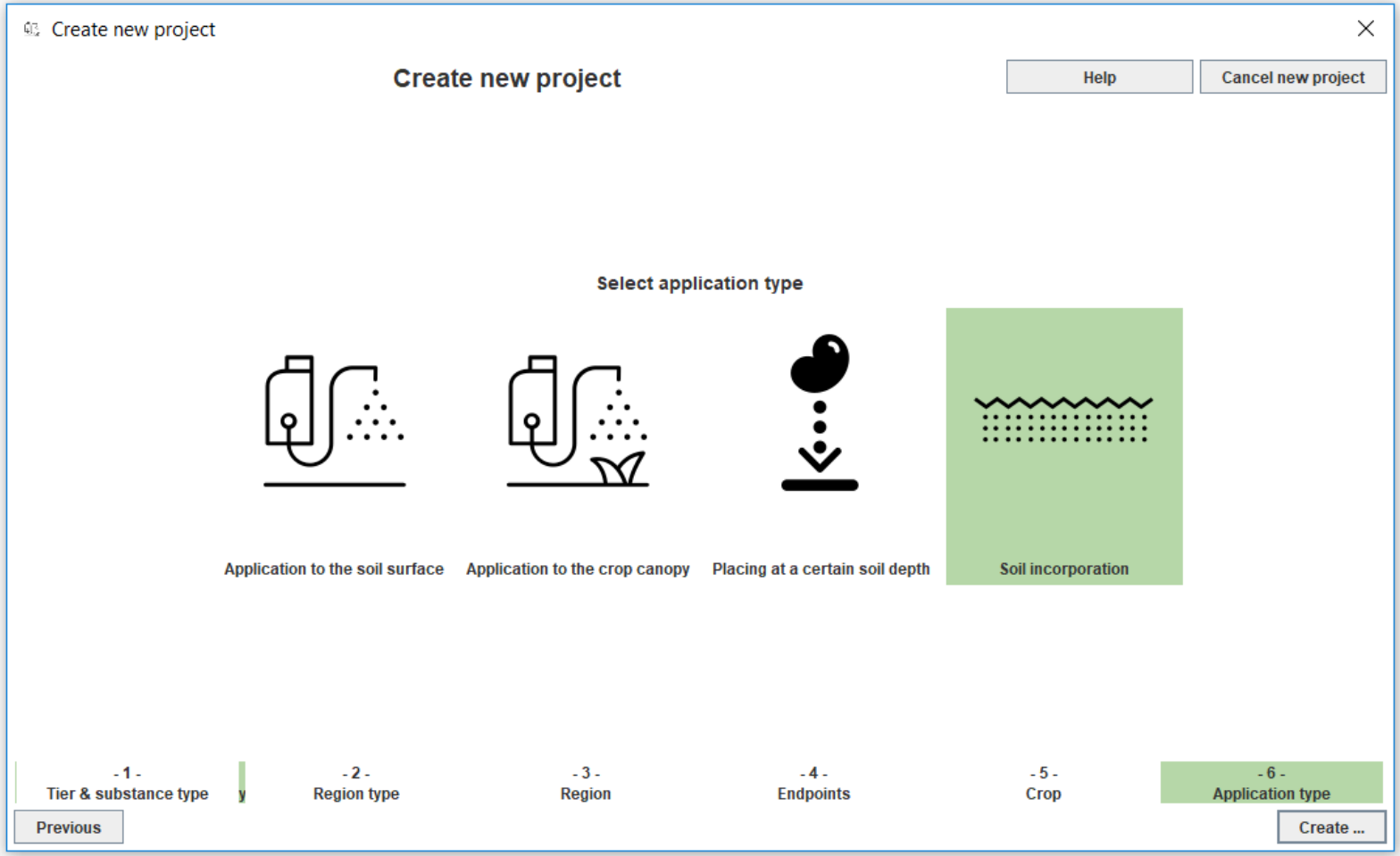
Tier 2. Evenly distributed incorporation of granules over a certain soil depth

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



Tier 2. Evenly distributed incorporation of granules over a certain soil depth

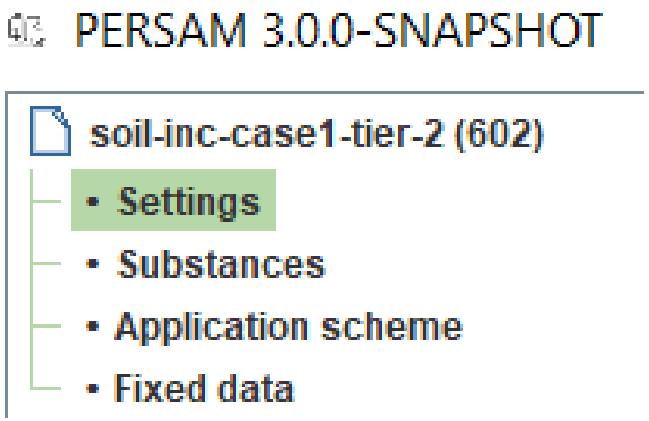
At **Tier 2** different types of application can be selected

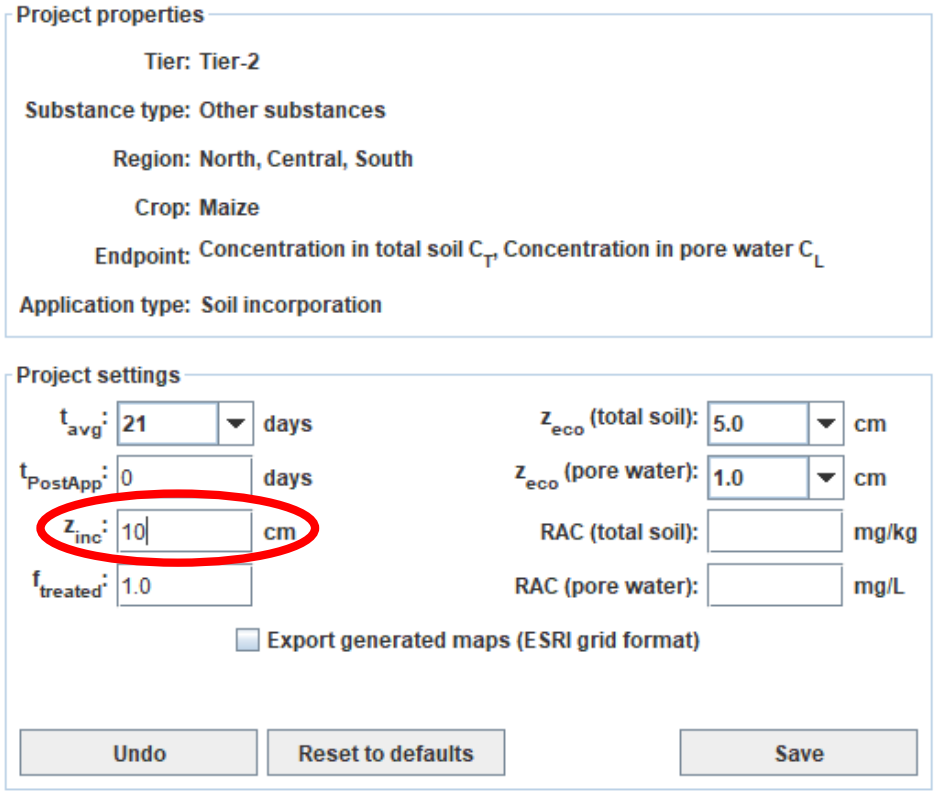


Tier 2. Evenly distributed incorporation of granules over a certain soil depth

Scenario parameterisation

Incorporation depth **(z_{inc})** can be set at **Tier 2**

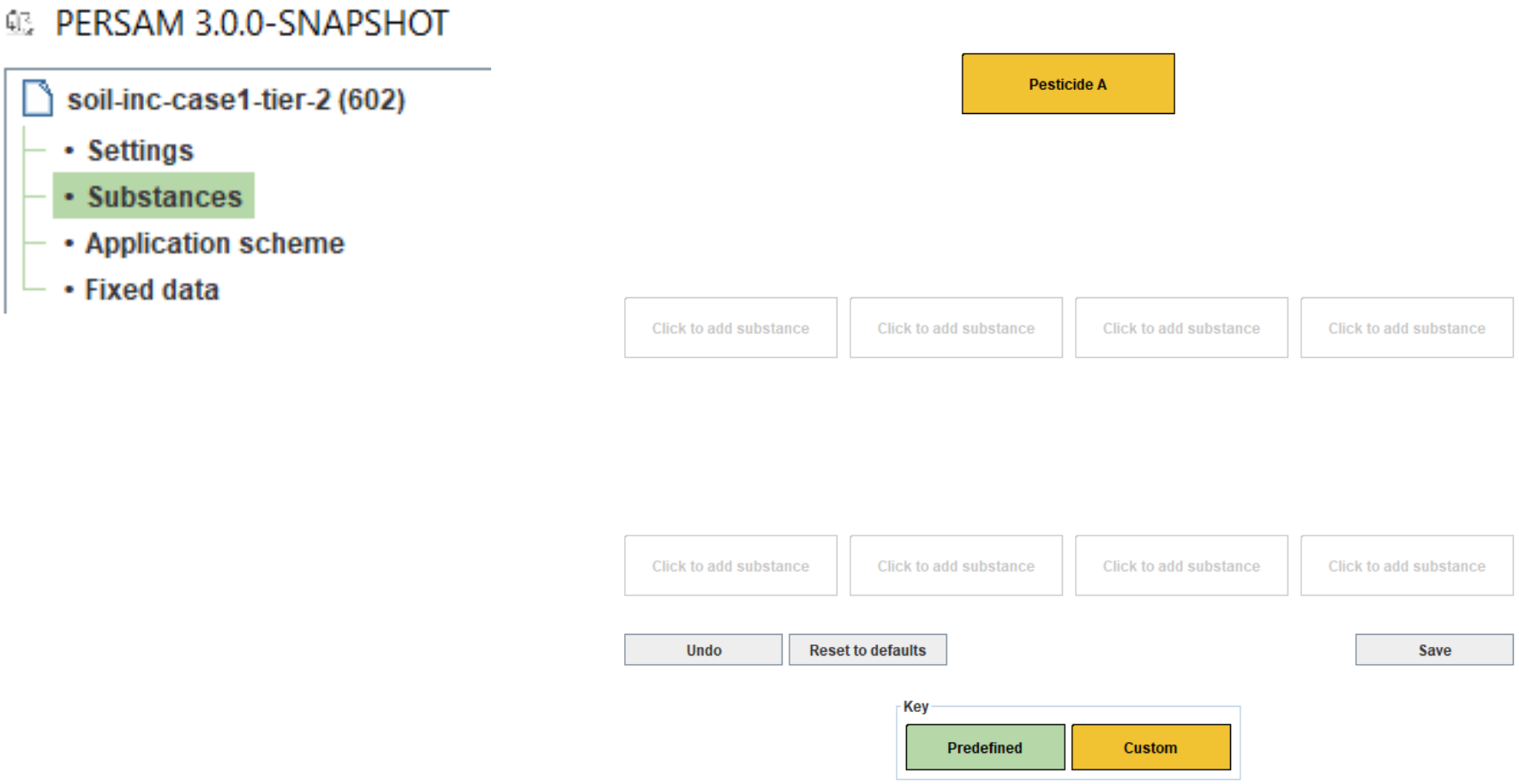




Tier 2. Evenly distributed incorporation of granules over a certain soil depth

Pesticide input parameters

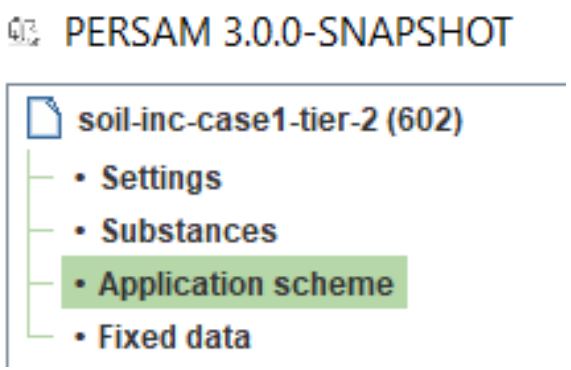
Degradation pathway (no metabolites considered)

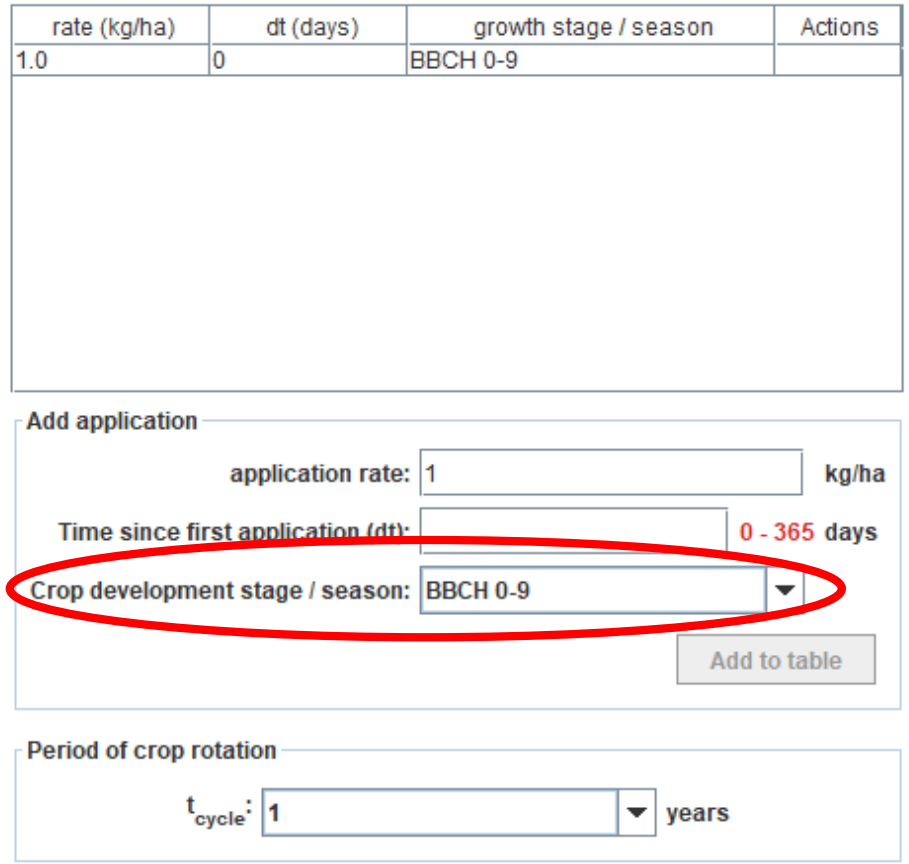


Tier 2. Evenly distributed incorporation of granules over a certain soil depth

Application scheme

At **Tier 2** crop interception is taken into account by setting the appropriate crop development stage (BBCH code) from *EFSA Guidance, 2014*.

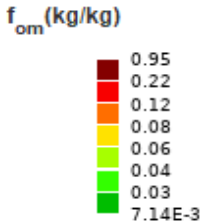




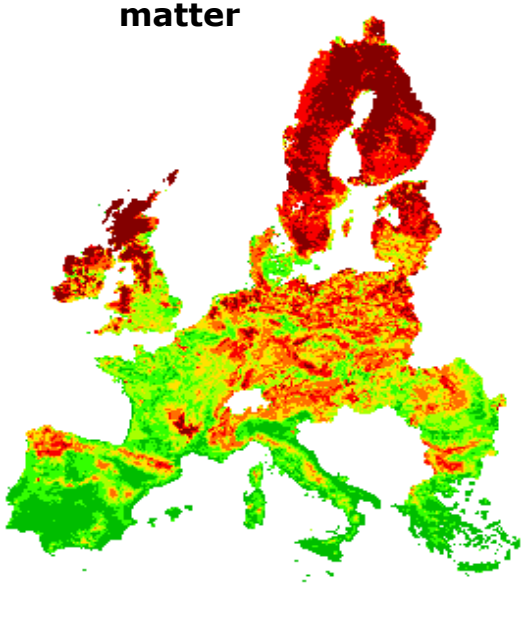
Tier 2. Evenly distributed incorporation of granules over a certain soil depth

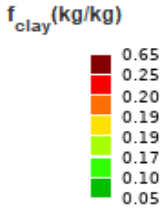
Fixed parameters

At **Tier 2** spatially distributed soil maps (1 km x 1 km pixel) are provided for soil properties

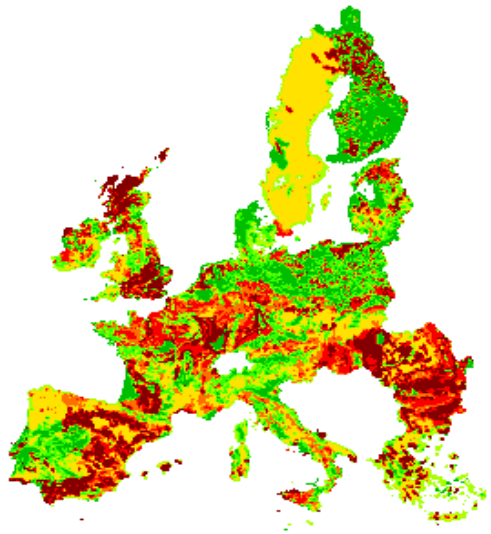


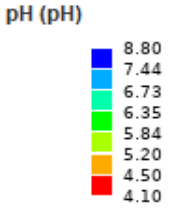
Fraction of organic matter



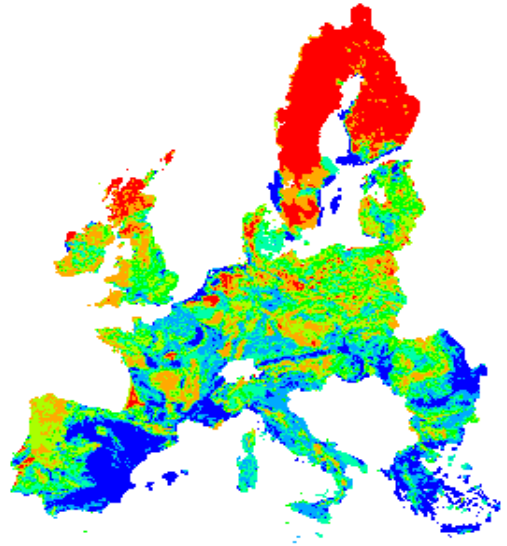


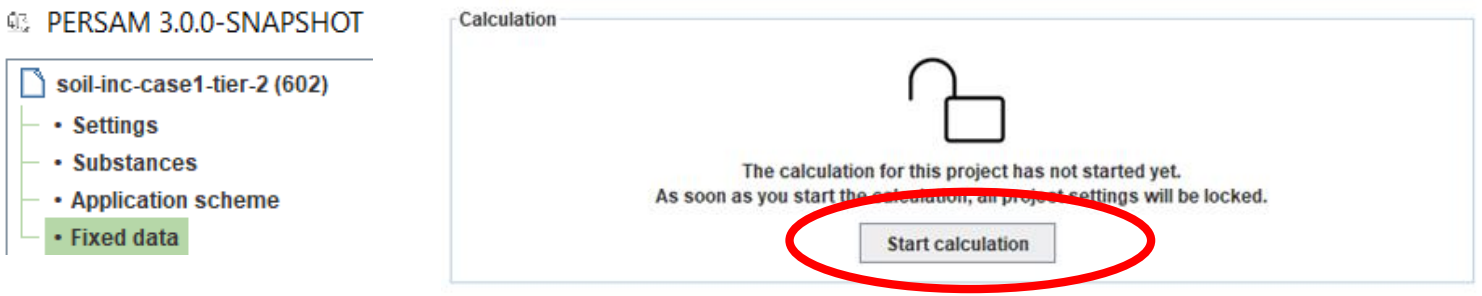
Fraction of clay



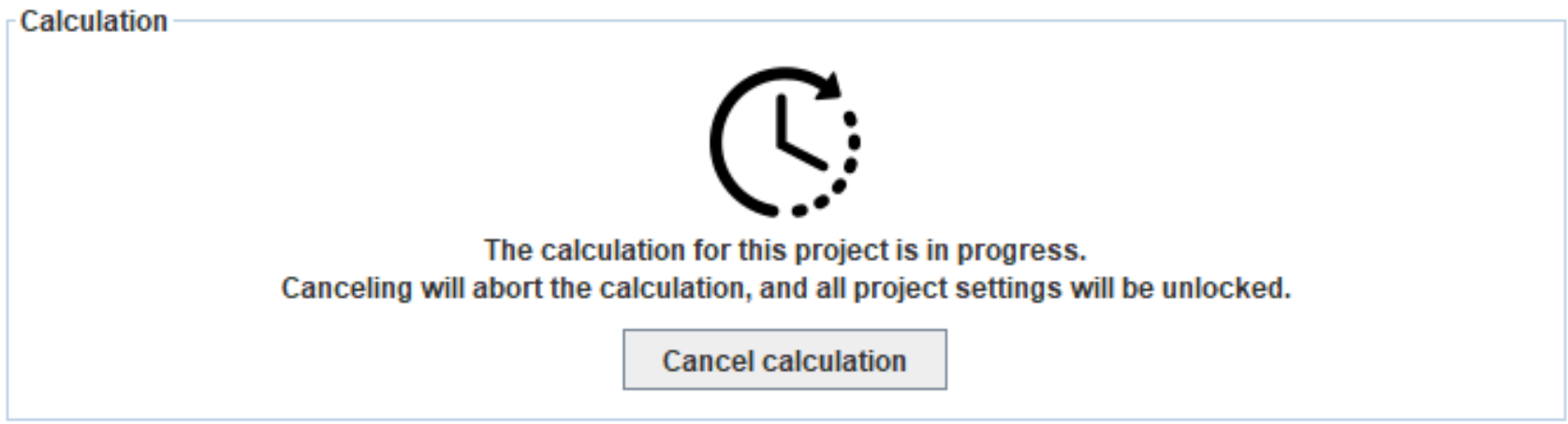


pH





Tier 2. Evenly distributed incorporation of granules over a certain soil depth

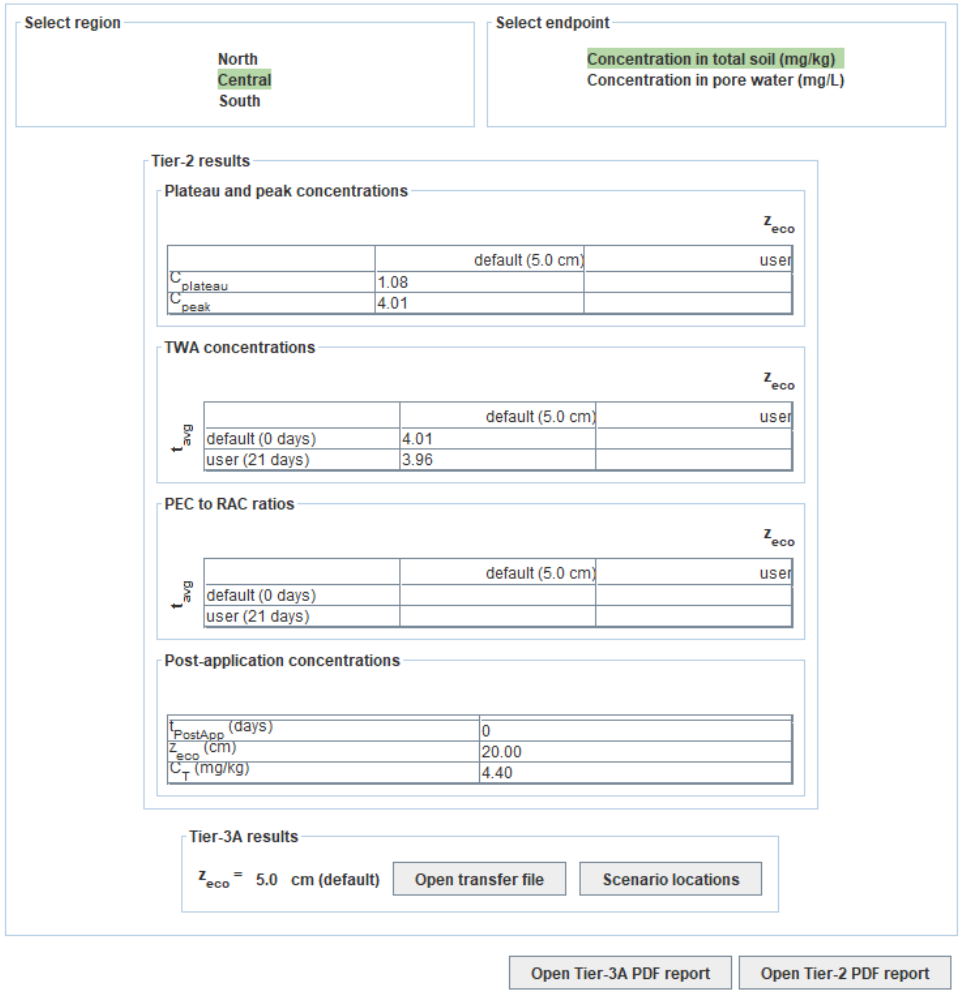


Tier 2. Evenly distributed incorporation of granules over a certain soil depth

Model output

Results of **Tier 2**

Generation of transfer file for Tier 3A assessment



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

z_{eco}

	default (5.0 cm)	user
$C_{plateau}$	1.08	
C_{peak}	4.01	

TWA concentrations

z_{eco}

t_{Ave}	default (5.0 cm)	user
default (0 days)	4.01	
user (21 days)	3.96	

PEC to RAC ratios

z_{eco}

t_{Ave}	default (5.0 cm)	user
default (0 days)		
user (21 days)		

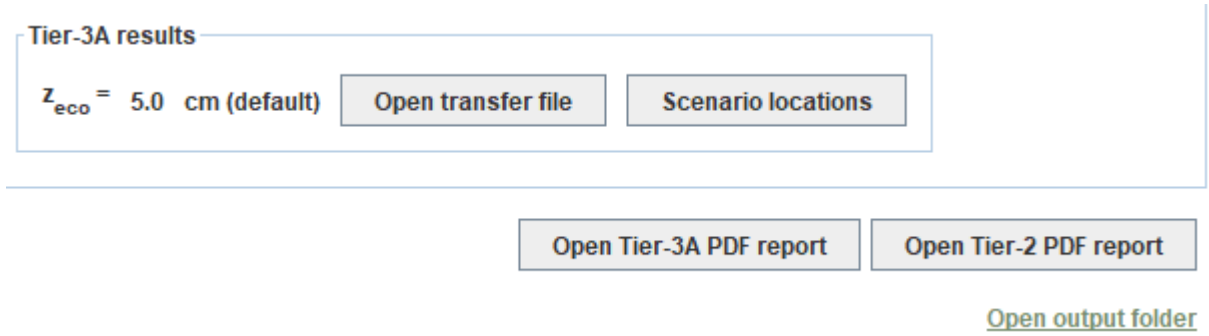
Post-application concentrations

$t_{PostApp}$ (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



Tier-3A results

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

Open Tier-3A PDF report Open Tier-2 PDF report

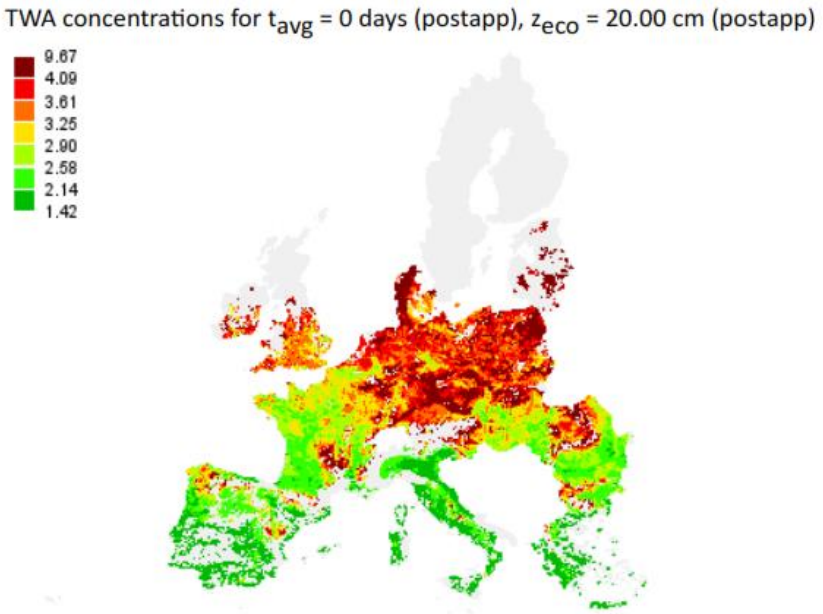
Open output folder

Tier 2. Evenly distributed incorporation of granules over a certain soil depth

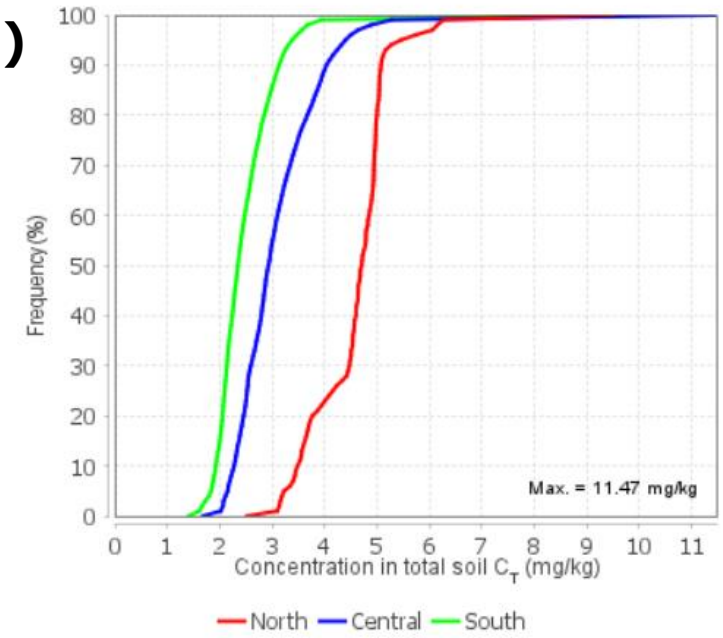
Model output: results of Tier 2

1) Spatially distributed PECs in soil for all regulatory zones
2) Frequency distributions of PECs in soil
3) Tables with TWA concentrations for single zones (Central)

1)



2)



3) *TWA concentrations*

Central Europe		z_{eco}	
		default (5.00 cm)	user
t_{avg}	default (0 days)	4.01 mg/kg	
	user (21 days)	3.96 mg/kg	

Tier 2. Placing of granules at a certain soil depth

Crop:
Maize

Number of applications:
1 application (1 kg/ha)

Type of application:
Granules are placed at a soil depth (z_{inc}) of 10 cm

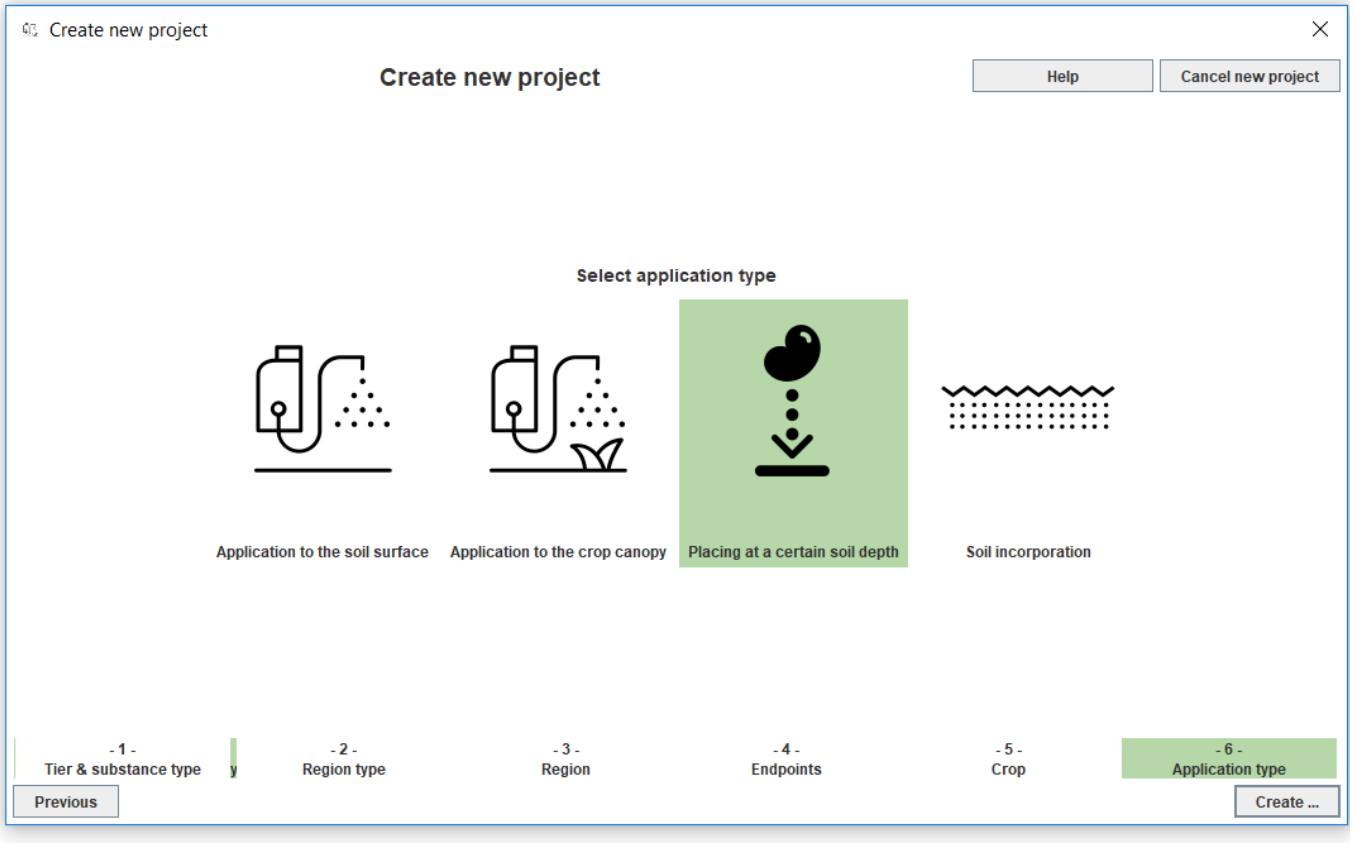
Time of application:
2 weeks before planting of maize (30 days before emergence)

Substance properties:
DegT50 (*geomean*): 250 days
Kom (*geomean*): 1000 (L/kg)
Molar mass: 300 g/mol
Water solubility: 0.1 mg/L

Substance property	Unit	A
Molar mass	(g/mol)	300
Water solubility (20°C)	(mg/L)	0.1
Vapour pressure (20°C)	(Pa)	10^{-8}
DegT50[(a)] (geomean)	(days)	250
Molar activation energy	(kJ/ mol^{-1})	65.4
Exponent for the effect of liquid	(–)	0.7
K_{om} (geomean)	(L/kg)	1,000
K_{om} in dry soil[(e)]	(L/kg)	10^5
1/*n*	(–)	0.9
DegT50 on crop surface	[(d)]	10
Wash-off factor[(g)]	(mm^{-1})	0.1
Plant uptake factor	(–)	0
Molar formation fraction (arithmetic mean)	(–)	–

Tier 2. Placing of granules at a certain soil depth

Scenario parameterisation



Project properties

Tier: Tier-2

Substance type: Other substances

Region: North, Central, South

Crop: Maize

Endpoint: Concentration in total soil C_T, Concentration in pore water C_L

Application type: Placing at a certain soil depth

Project settings

t_{avg}:	21 days	z_{eco} (total soil):	5.0 cm
$t_{PostApp}$:	0 days	z_{eco} (pore water):	1.0 cm
z_{inc}:	10 cm	RAC (total soil):	mg/kg
$f_{treated}$:	1.0	RAC (pore water):	mg/L

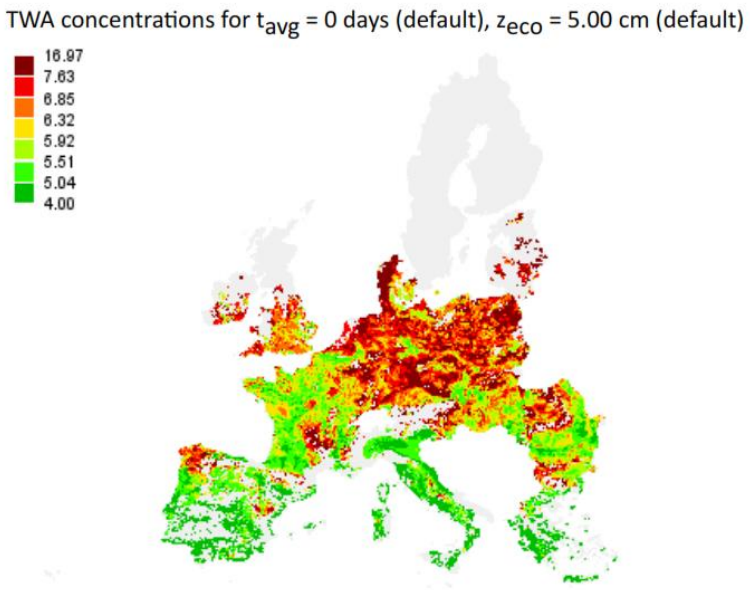
Export generated maps (ESRI grid format)

Undo | Reset to defaults | Save

Model output: results of Tier 2

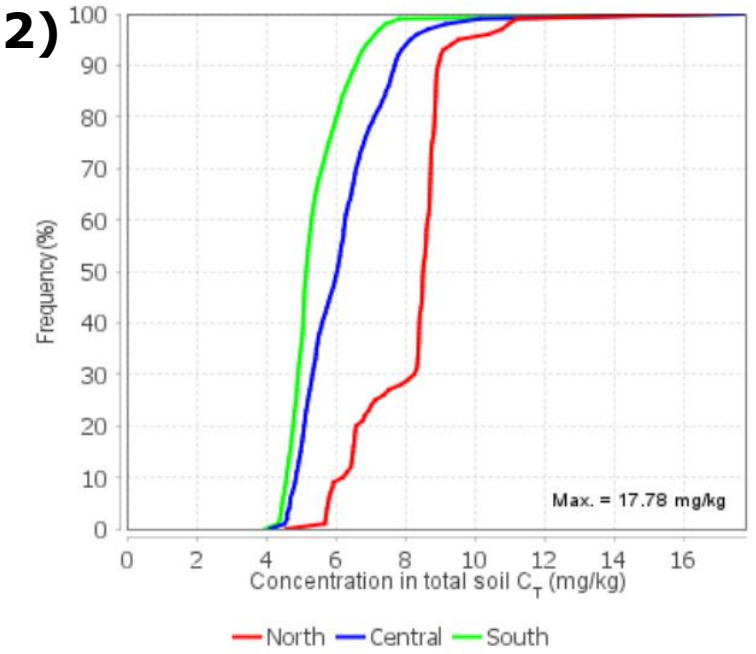
1) Spatially distributed PECs in soil for all regulatory zones
2) Frequency distributions of PECs in soil
3) Tables with TWA concentrations for single zones (Central)

1)



TWA concentrations

2)



3)

Central Europe		z_{eco}	
		default (5.00 cm)	user
t_{avg}	default (0 days)	8.16 mg/kg	
	user (21 days)	8.07 mg/kg	

TIER 3A modelling is performed with PEARL and PELMO

FOCUS PELMO (soil beta) will be used in the following worked-examples:

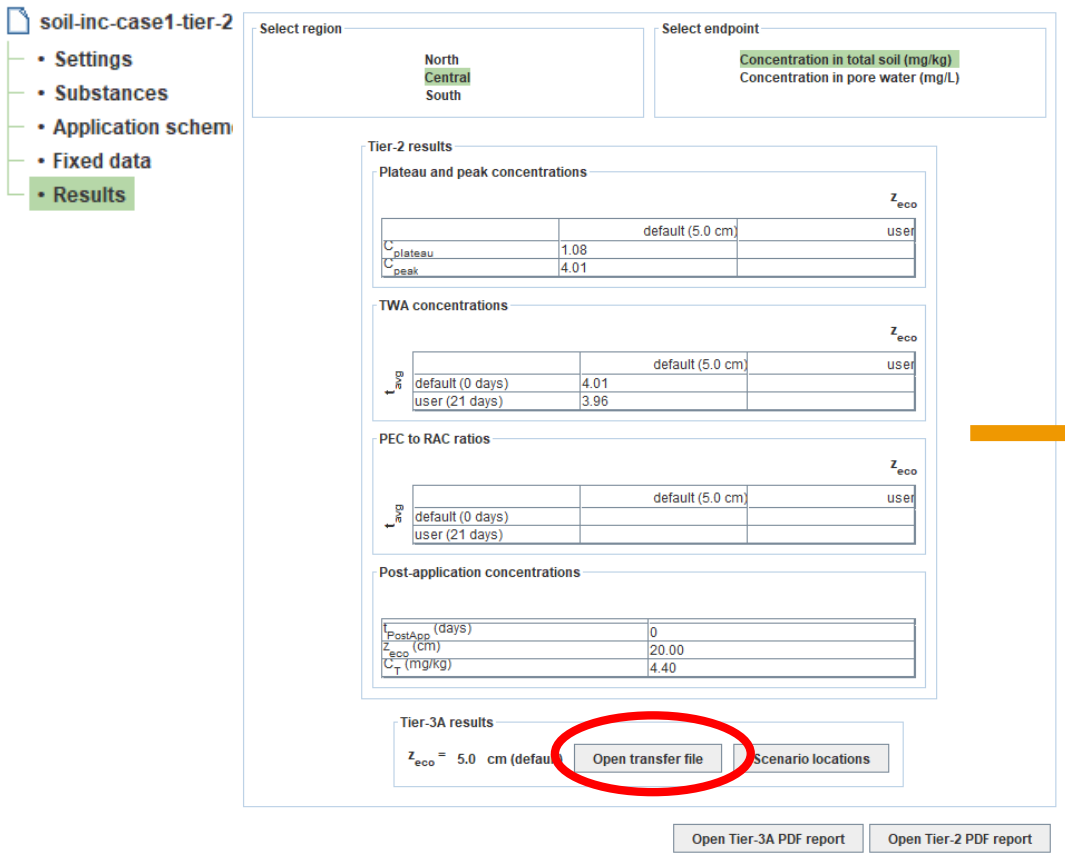
1) Evenly distributed incorporation of granules over a certain soil depth

2) Placing of granules at a certain soil depth

Higher tier assessment (Tier 3A)

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

PERSAM



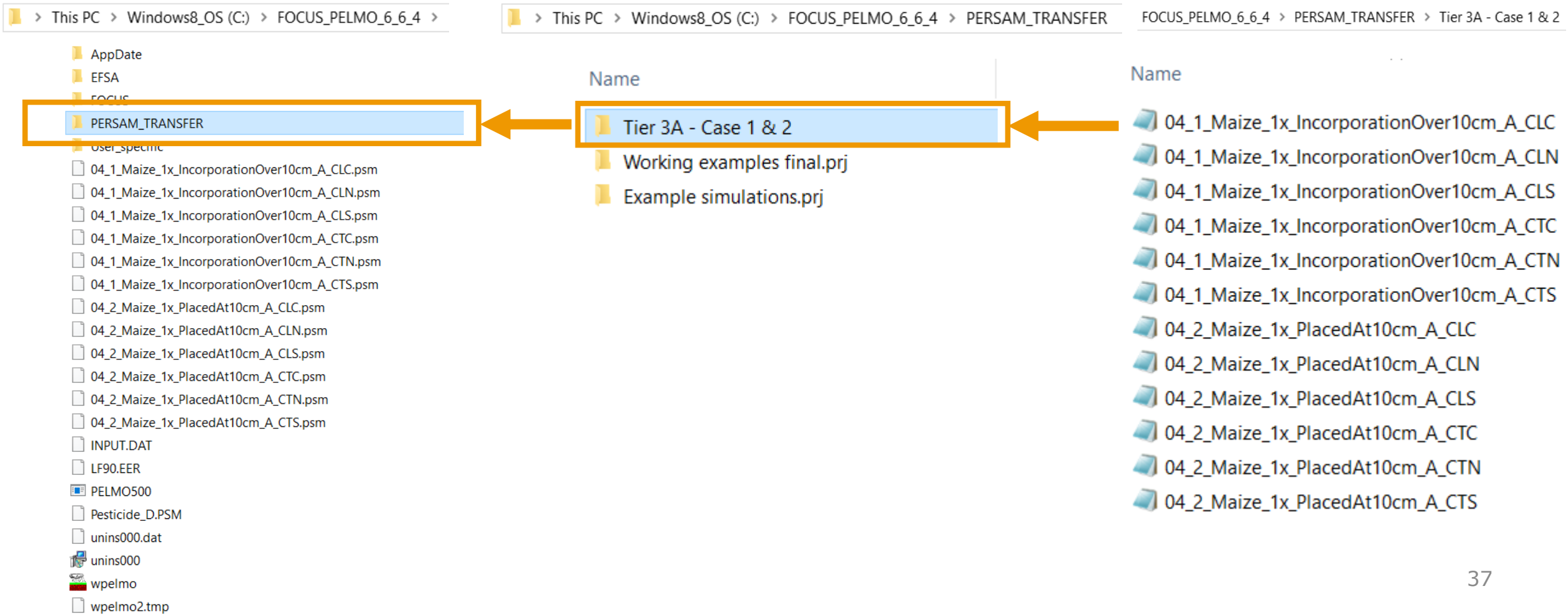
Transfer file (.ptf)

PELMO

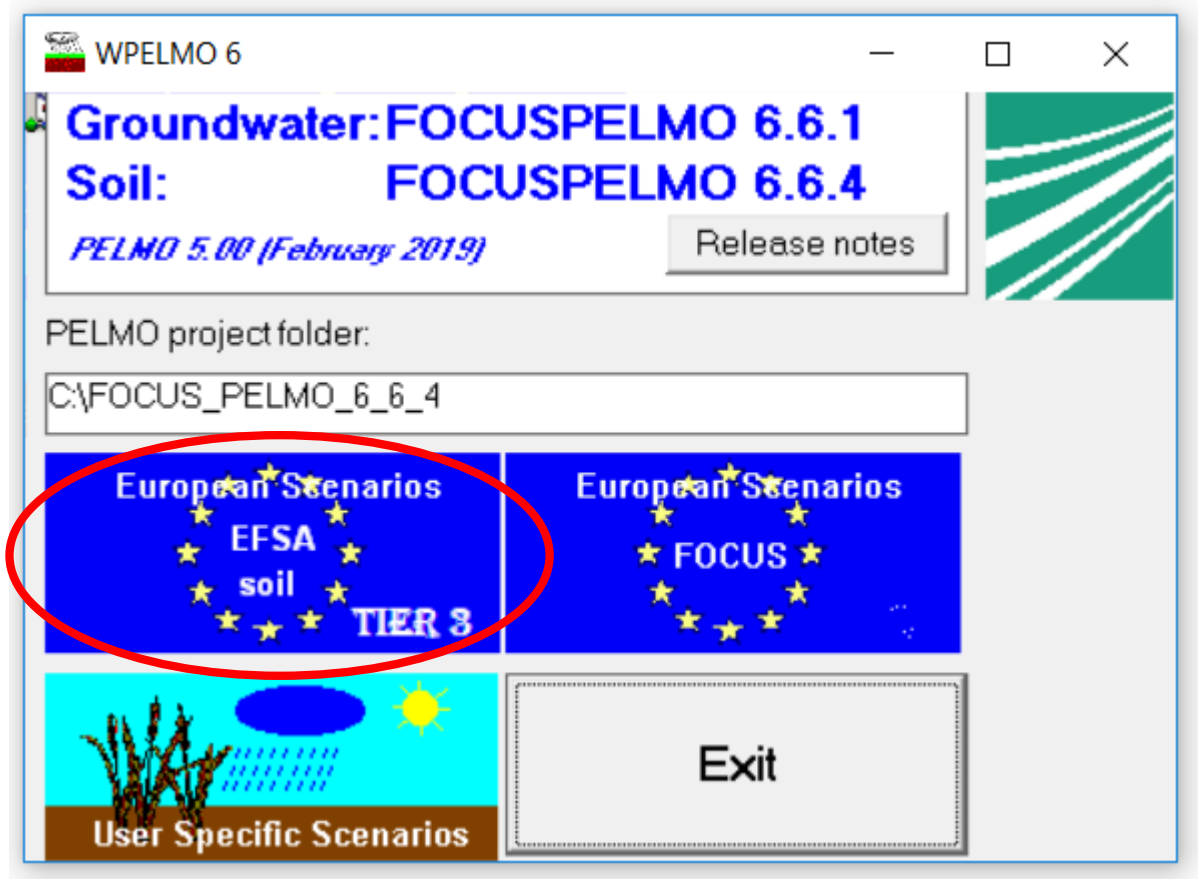
Higher tier assessment (Tier 3A) with FOCUS PELMO

PERSAM transfer files for selected scenarios have to be copied in **PELMO** folder

(*Case 1 & 2, North, Centre, South, PEC*$_{soil}$*, PEC*$_{pore\ water}$)



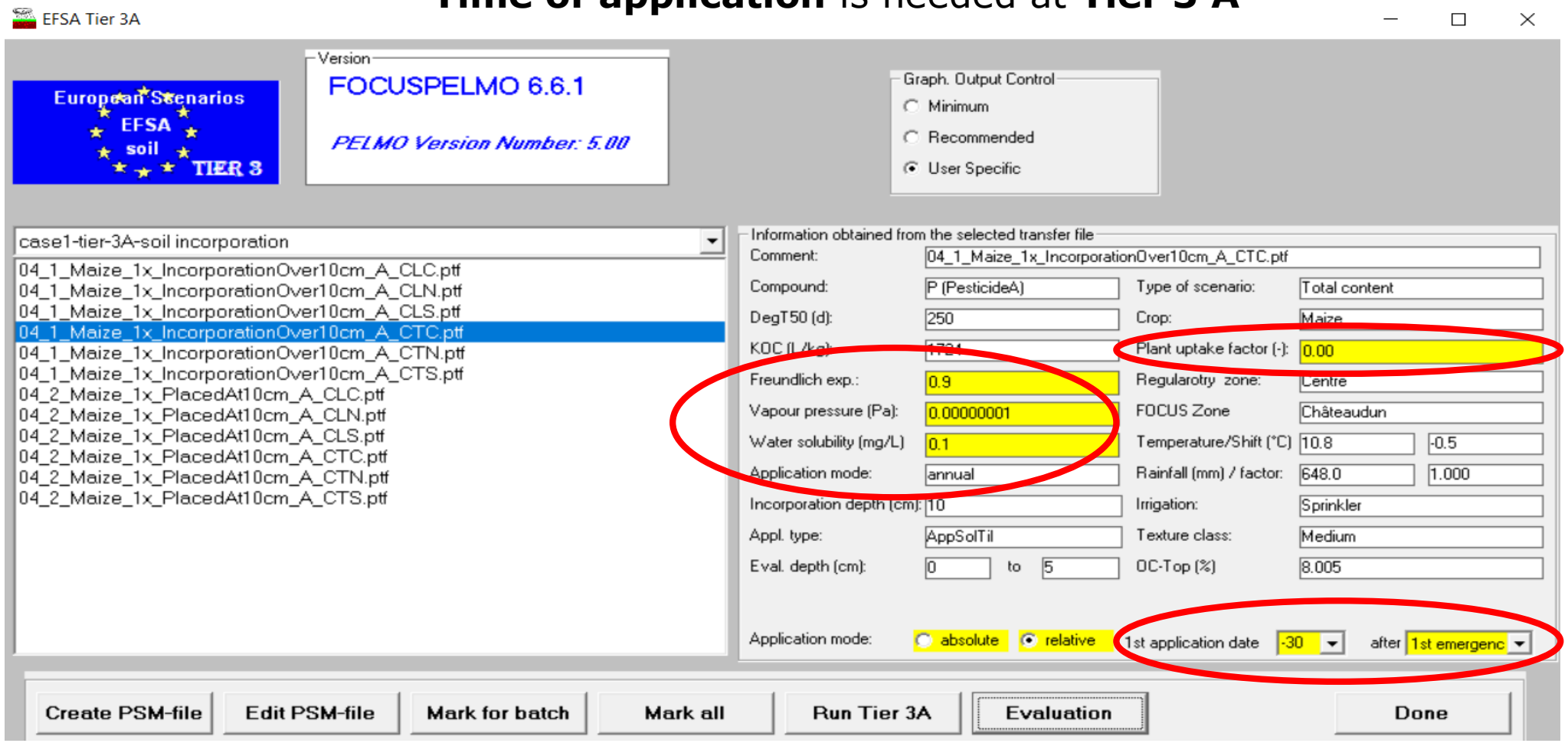
PELMO Graphical shell



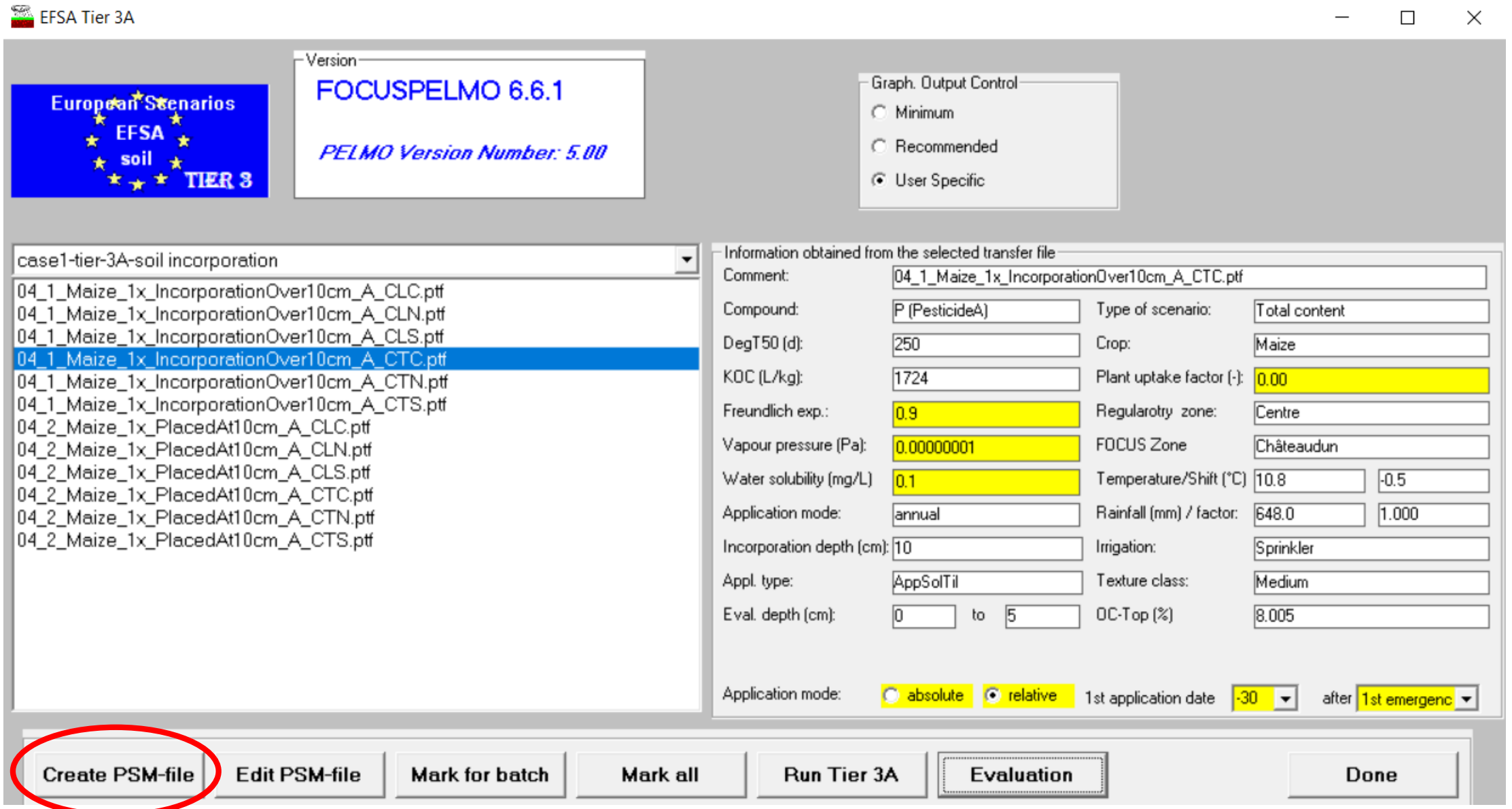
Tier 3A with PELMO: Evenly distributed incorporation of granules over a certain soil depth

Scenario refinement with PELMO

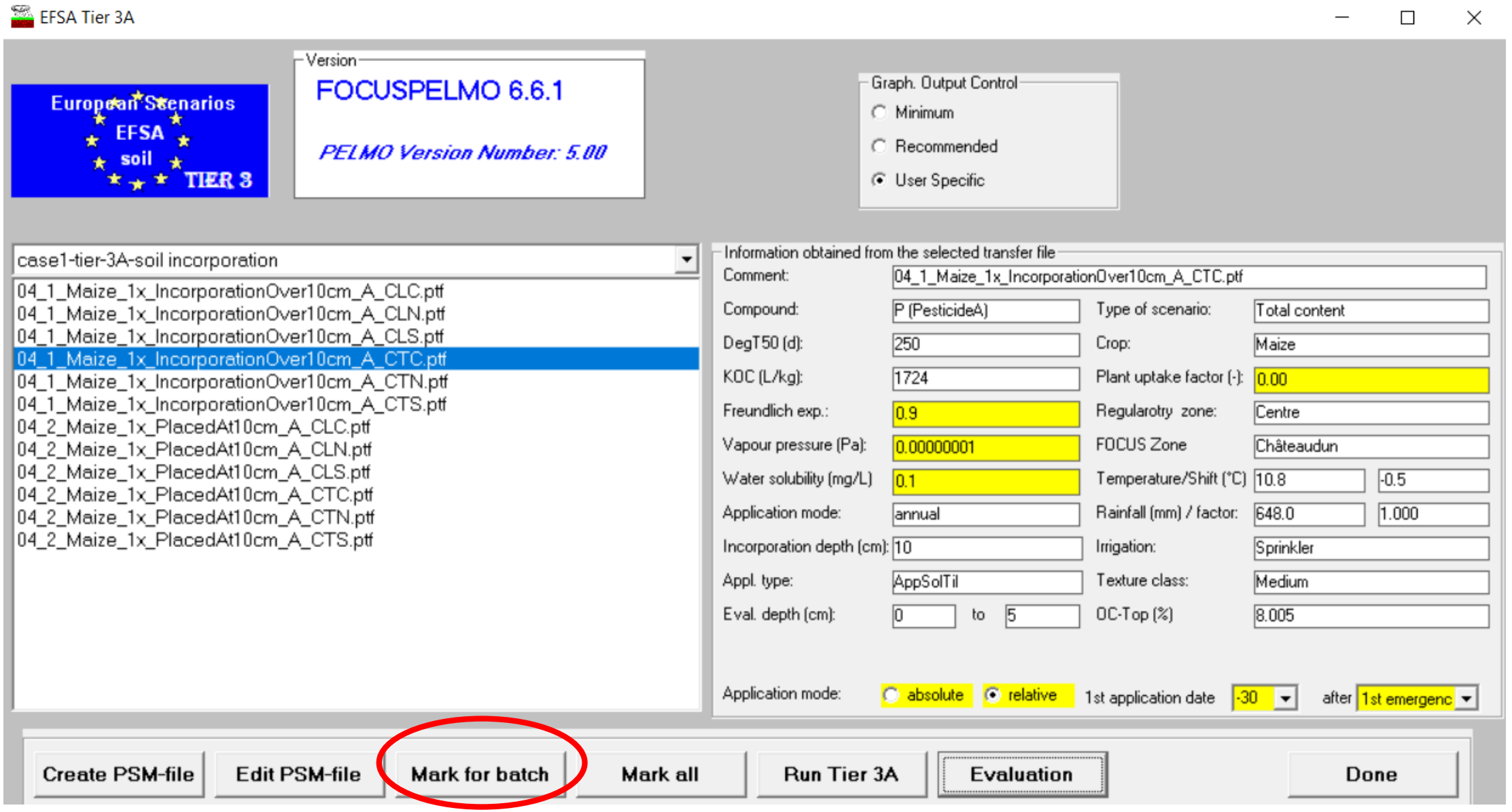
Further substance properties are required at **Tier 3 A**
Time of application is needed at **Tier 3 A**



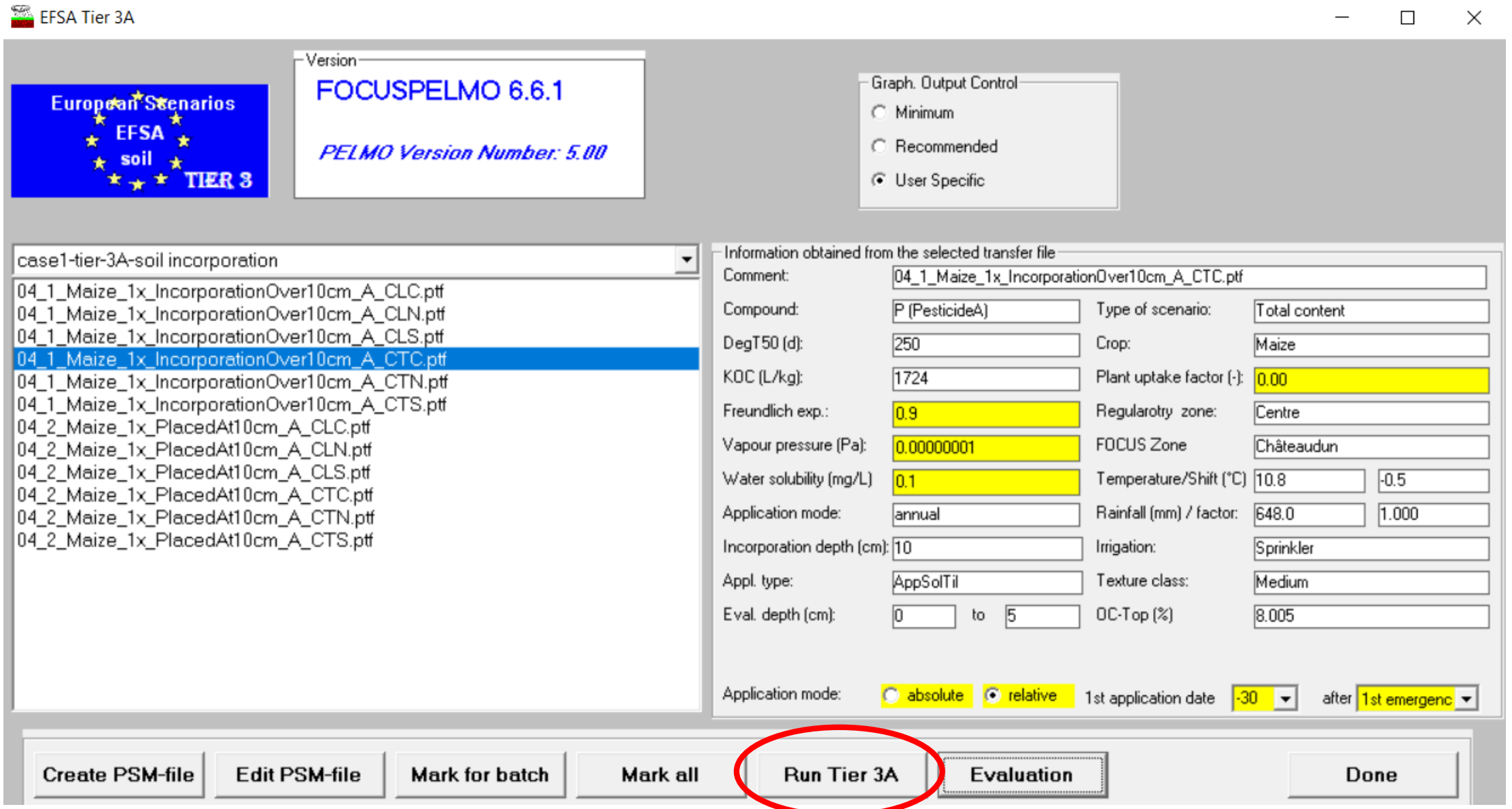
Tier 3A with PELMO: Evenly distributed incorporation of granules over a certain soil depth



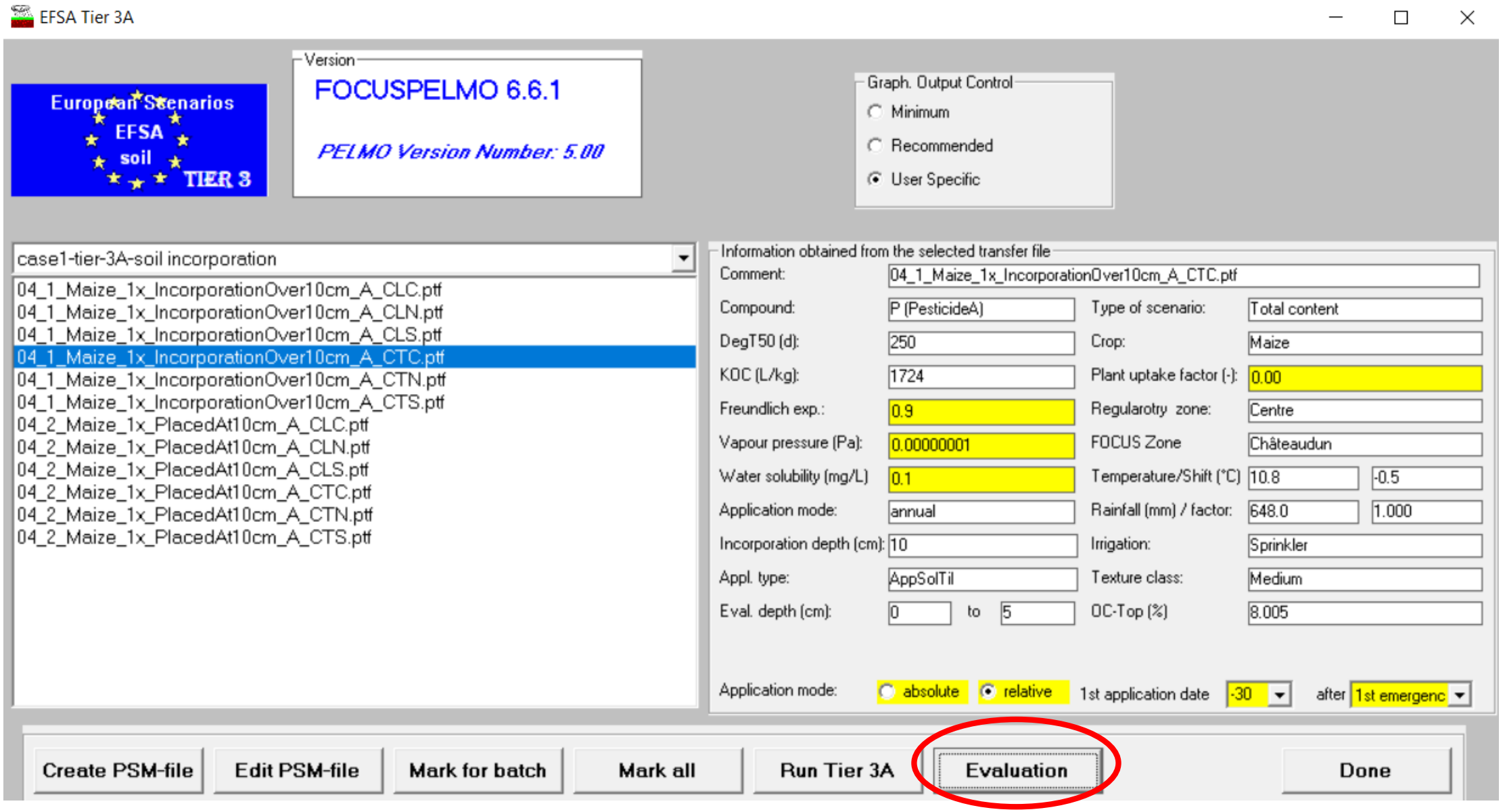
Tier 3A with PELMO: Evenly distributed incorporation of granules over a certain soil depth



Tier 3A with PELMO: Evenly distributed incorporation of granules over a certain soil depth



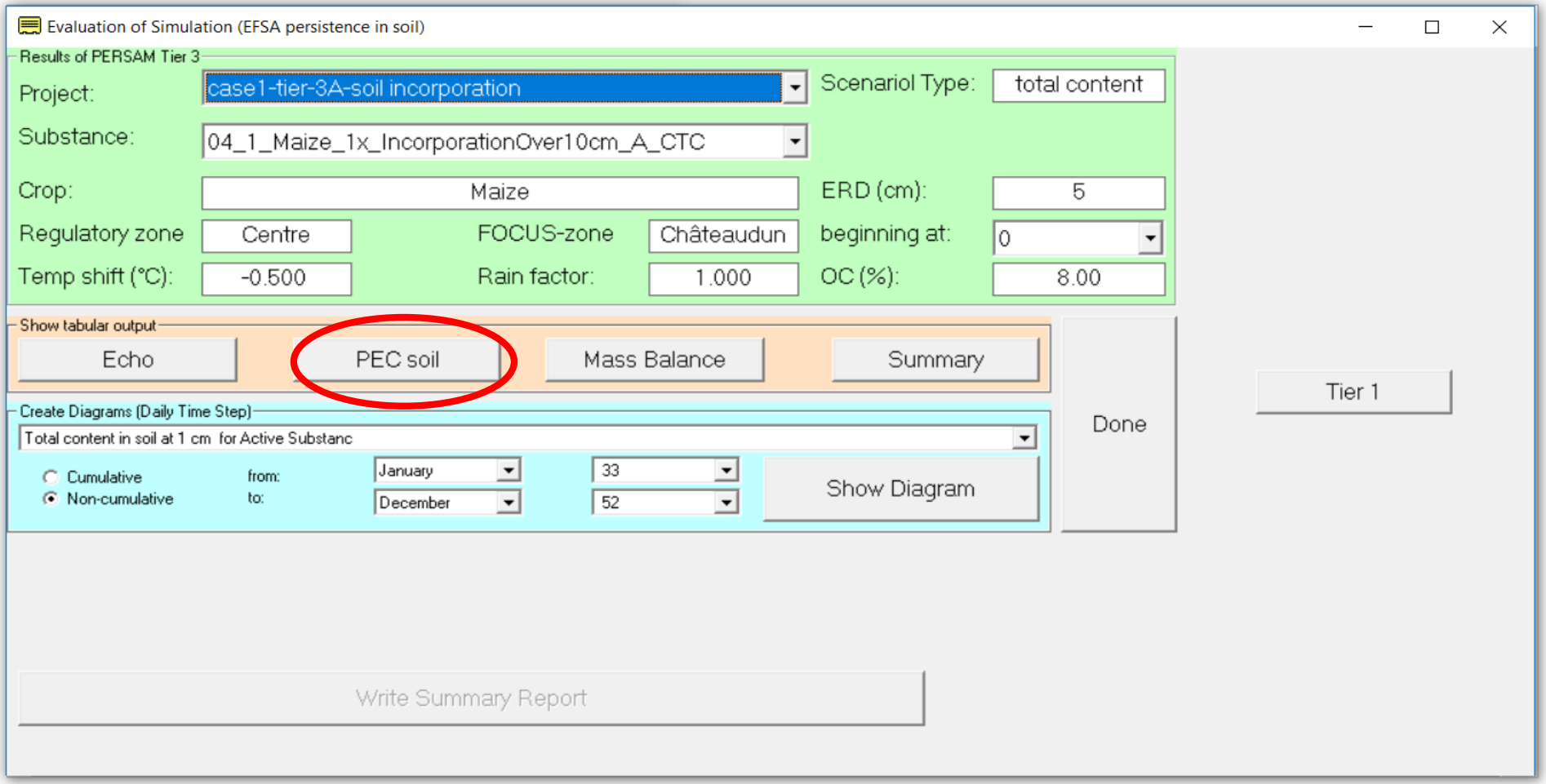
Tier 3A with PELMO: Evenly distributed incorporation of granules over a certain soil depth



Tier 3A with PELMO: Evenly distributed incorporation of granules over a certain soil depth

PECs in soil for single scenarios

Central Europe, soil incorporation

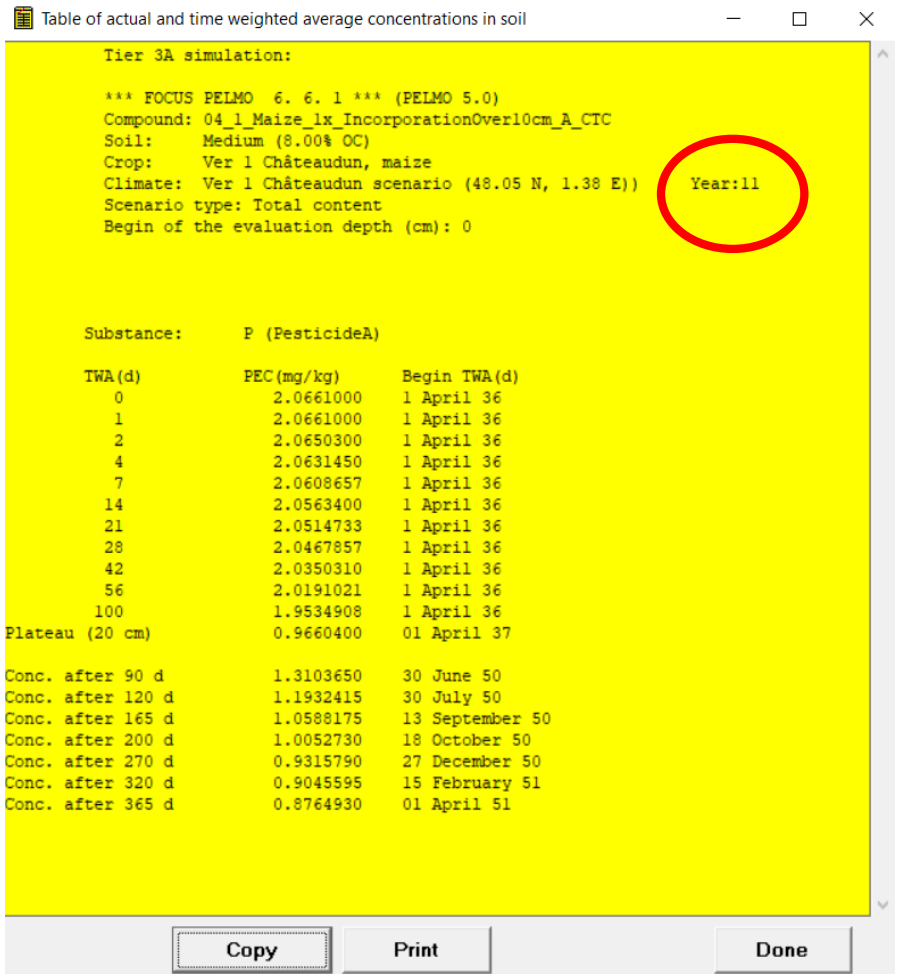


Tier 3A with PELMO: Evenly distributed incorporation of granules over a certain soil depth

Time weighted average (**TWA**) concentrations (mg/kg) over 100 days

Plateau concentration

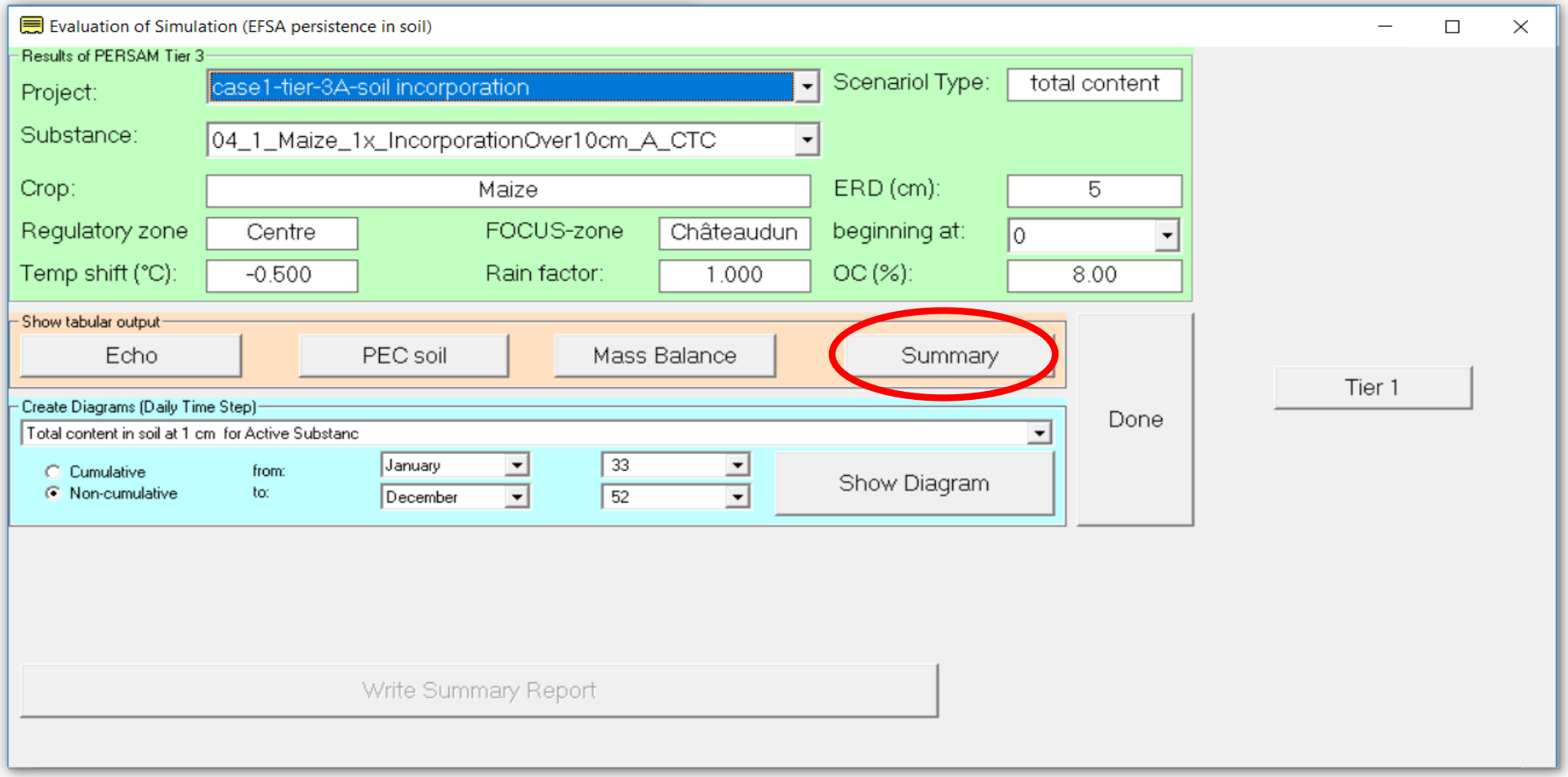
Concentrations post-application



Tier 3A with PELMO: Evenly distributed incorporation of granules over a certain soil depth

Results of Tier 3 with PELMO

Summary of all the modelled scenarios



Tier 3A with PELMO: Evenly distributed incorporation of granules over a certain soil depth

Summary of all the modelled scenarios

PECs in soil and pore water for North, Central and South Europe following soil incorporation and placing at certain soil depth

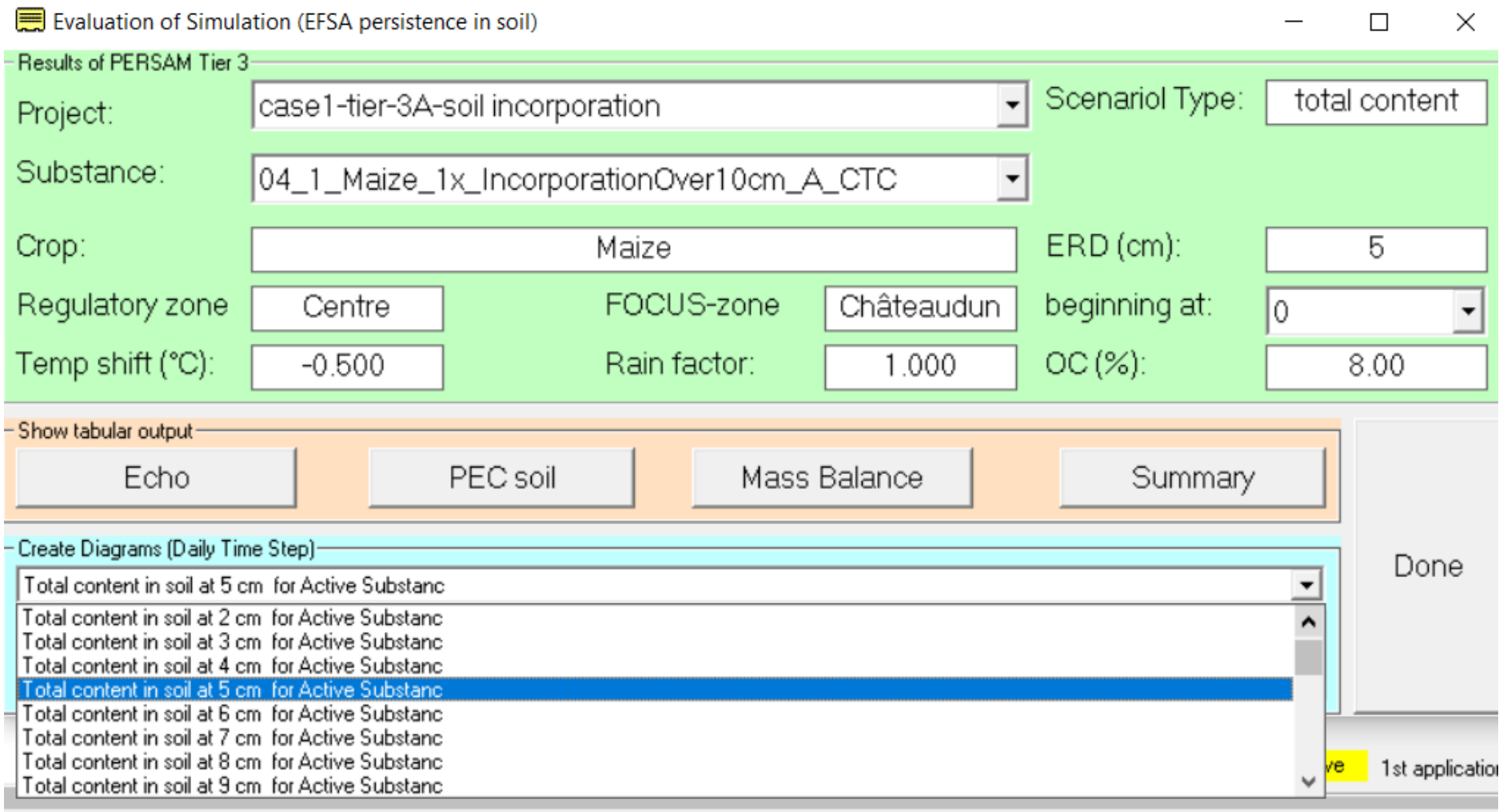
EFSA Summary Output File

Model Version: FOCUSPELMO 6.6.1
Project: Tier 3A - Case 1 & 2

Crop	Type	Zone	Substance/Situation	ERD (cm)	Conc. TWA0		Conc. TWA21	
Maize	pore water	2 Centre	04_1_Maize_1x_IncorporationOver10cm_A_CLC	1	0.056264	mg/L	0.0561101	mg/L
Maize	pore water	1 North	04_1_Maize_1x_IncorporationOver10cm_A_CLN	1	0.047692	mg/L	0.0464072	mg/L
Maize	pore water	3 South	04_1_Maize_1x_IncorporationOver10cm_A_CLS	1	0.069915	mg/L	0.0668131	mg/L
Maize	total content	2 Centre	04_1_Maize_1x_IncorporationOver10cm_A_CTC	5	2.0661	mg/kg	2.0514733	mg/kg
Maize	total content	1 North	04_1_Maize_1x_IncorporationOver10cm_A_CTN	5	2.72812	mg/kg	2.7120971	mg/kg
Maize	total content	3 South	04_1_Maize_1x_IncorporationOver10cm_A_CTS	5	1.74202	mg/kg	1.7270286	mg/kg
Maize	pore water	2 Centre	04_2_Maize_1x_PlacedAt10cm_A_CLC	1	0.41712	mg/L	0.4131061	mg/L
Maize	pore water	1 North	04_2_Maize_1x_PlacedAt10cm_A_CLN	1	0.380727	mg/L	0.3767733	mg/L
Maize	pore water	3 South	04_2_Maize_1x_PlacedAt10cm_A_CLS	1	0.46655	mg/L	0.4591229	mg/L
Maize	total content	2 Centre	04_2_Maize_1x_PlacedAt10cm_A_CTC	5	3.624282	mg/kg	3.6014895	mg/kg
Maize	total content	1 North	04_2_Maize_1x_PlacedAt10cm_A_CTN	5	4.837312	mg/kg	4.803682	mg/kg
Maize	total content	3 South	04_2_Maize_1x_PlacedAt10cm_A_CTS	5	2.856076	mg/kg	2.8259359	mg/kg

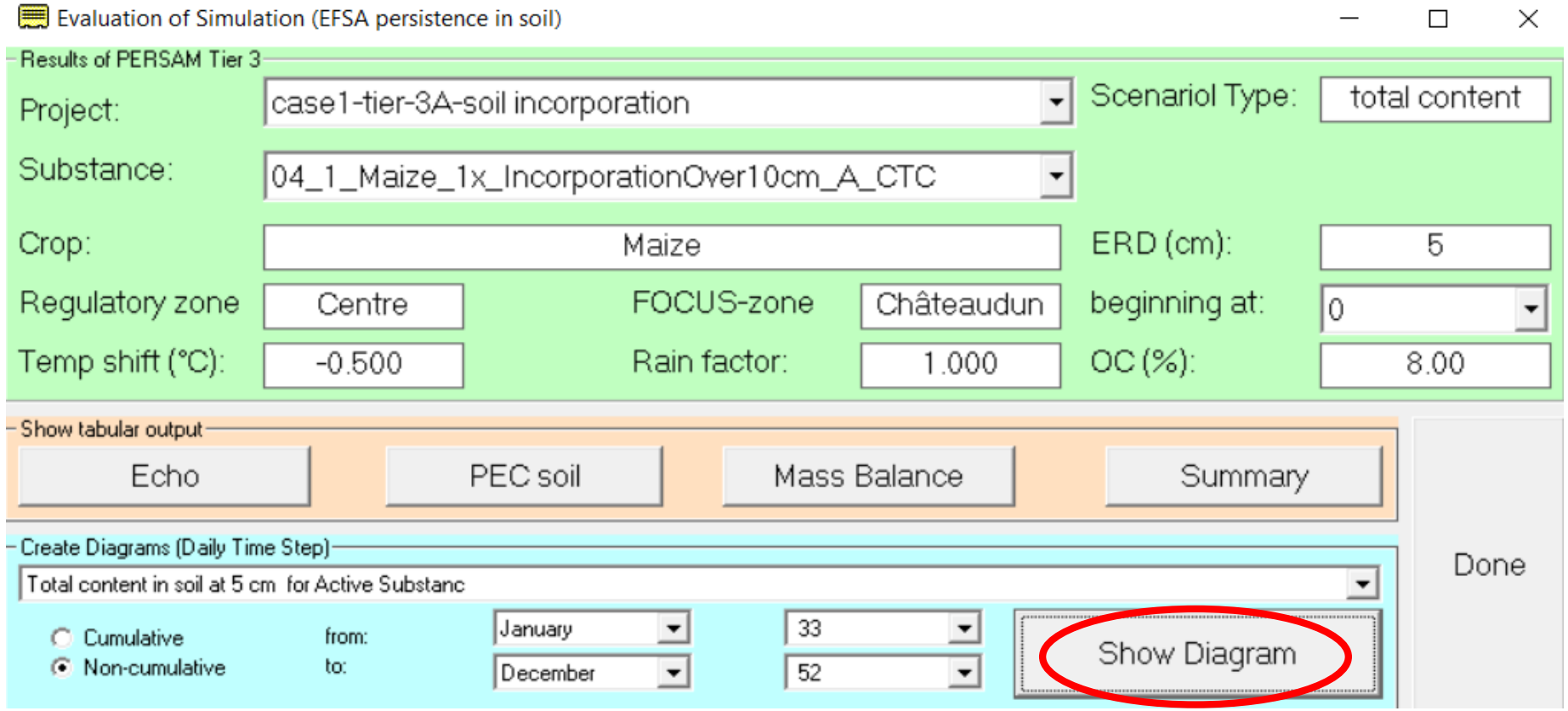
Tier 3A with PELMO: Evenly distributed incorporation of granules over a certain soil depth

Graphical output



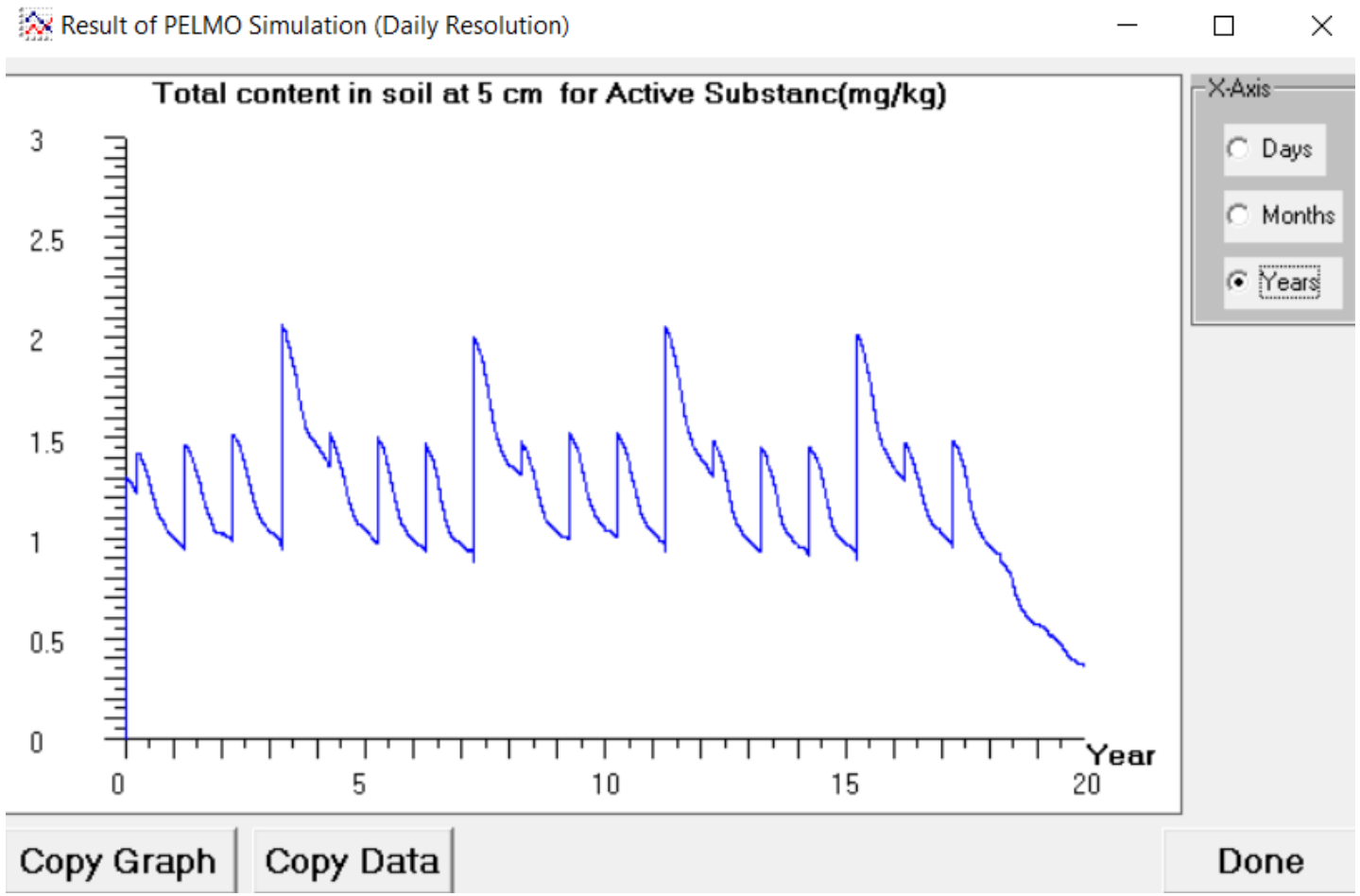
Tier 3A with PELMO: Evenly distributed incorporation of granules over a certain soil depth

Graphical output



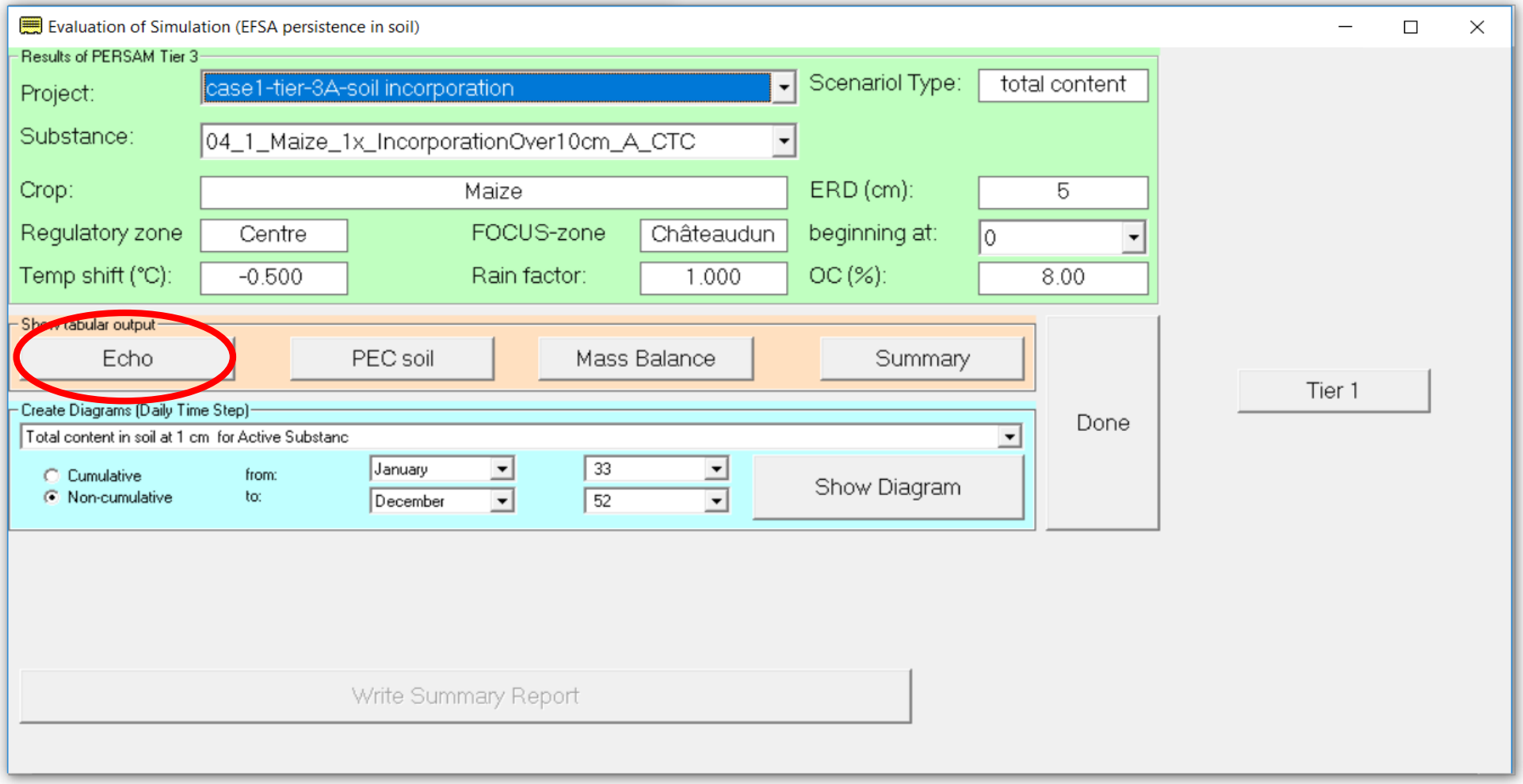
Tier 3A with PELMO: Evenly distributed incorporation of granules over a certain soil depth

Graphical output



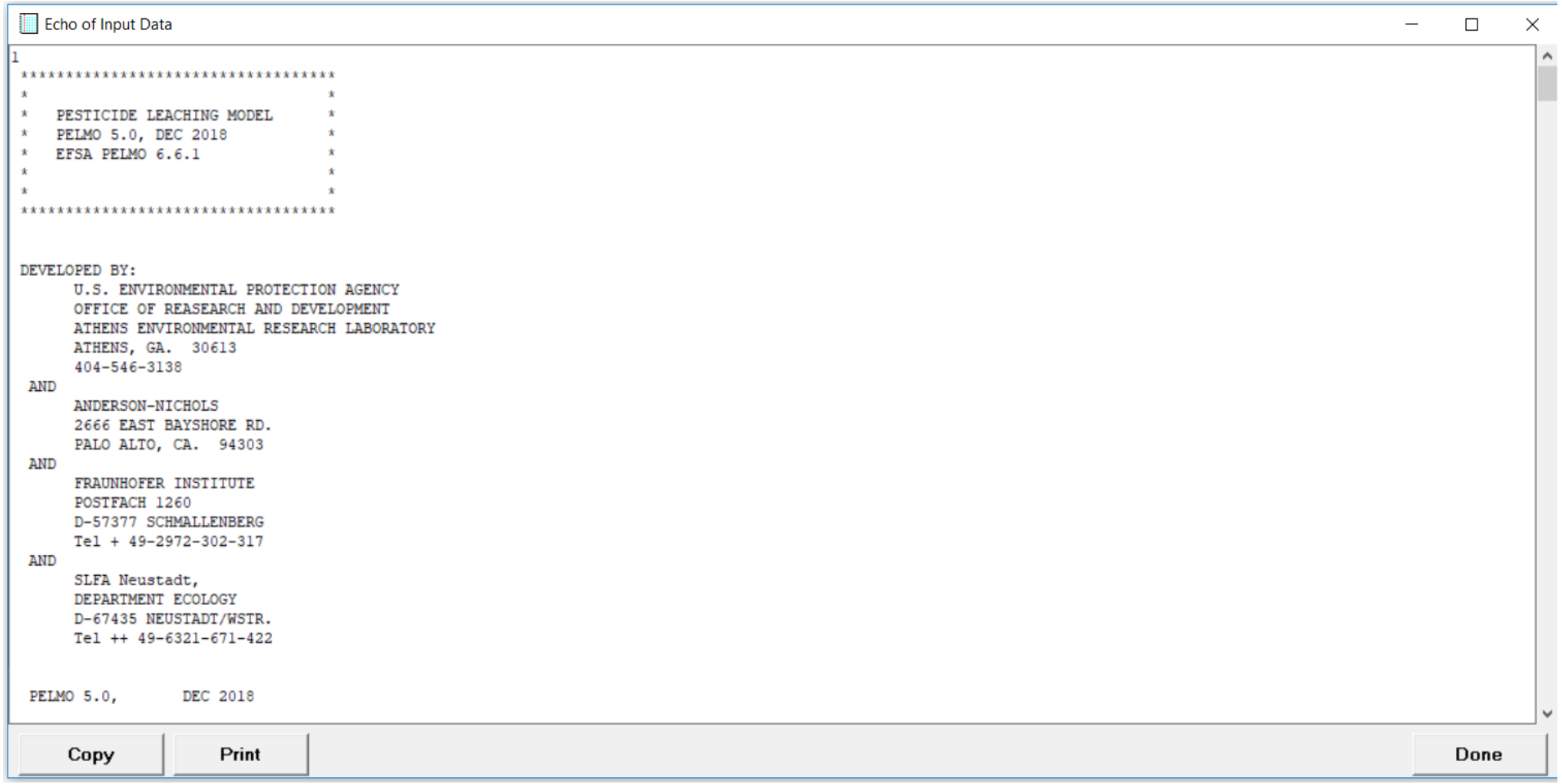
Tier 3A with PELMO: Evenly distributed incorporation of granules over a certain soil depth

Display model parameters



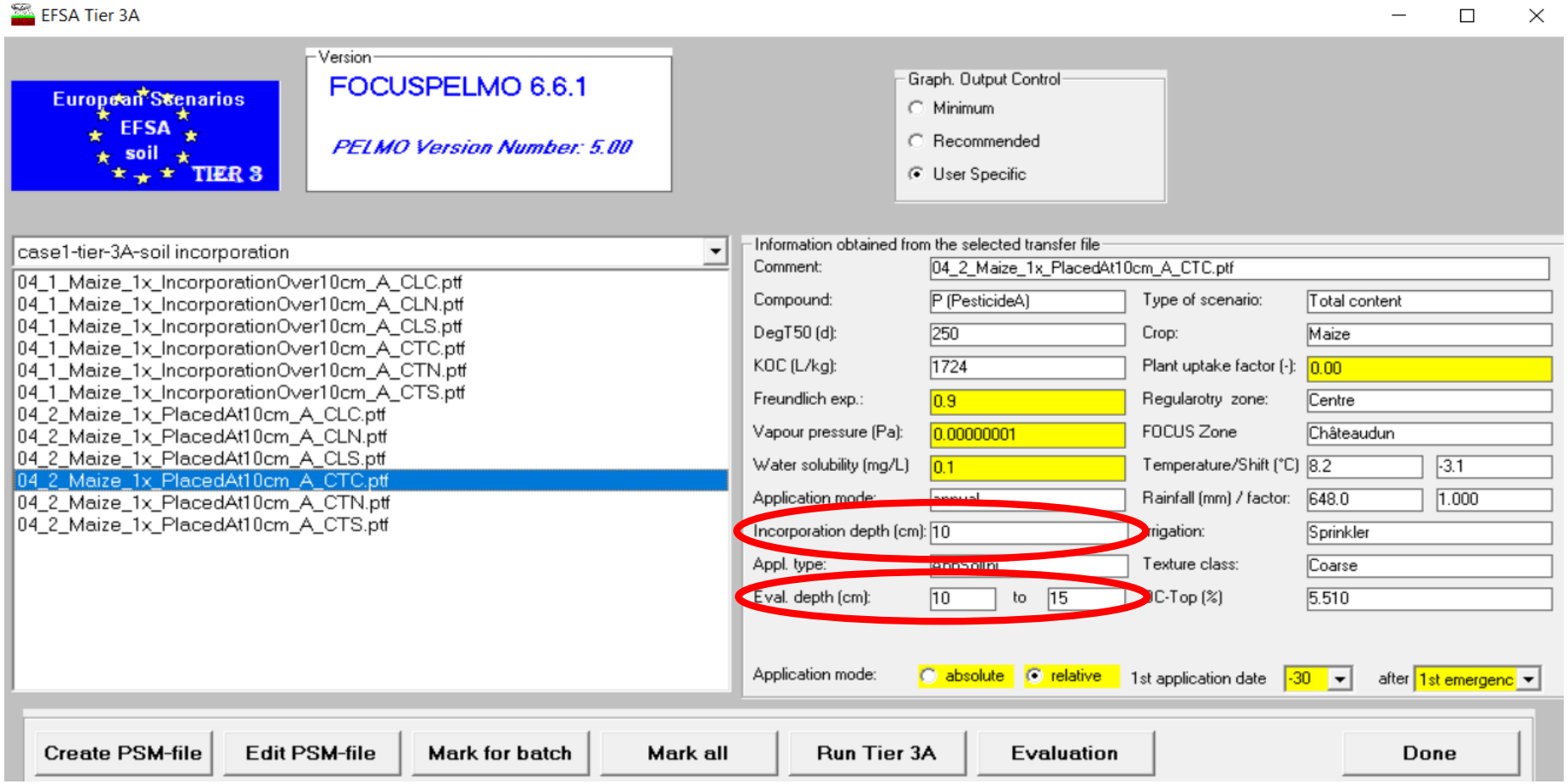
Tier 3A with PELMO: Evenly distributed incorporation of granules over a certain soil depth

Display model parameters



Case 2 : placing at certain soil depth

Input parameters



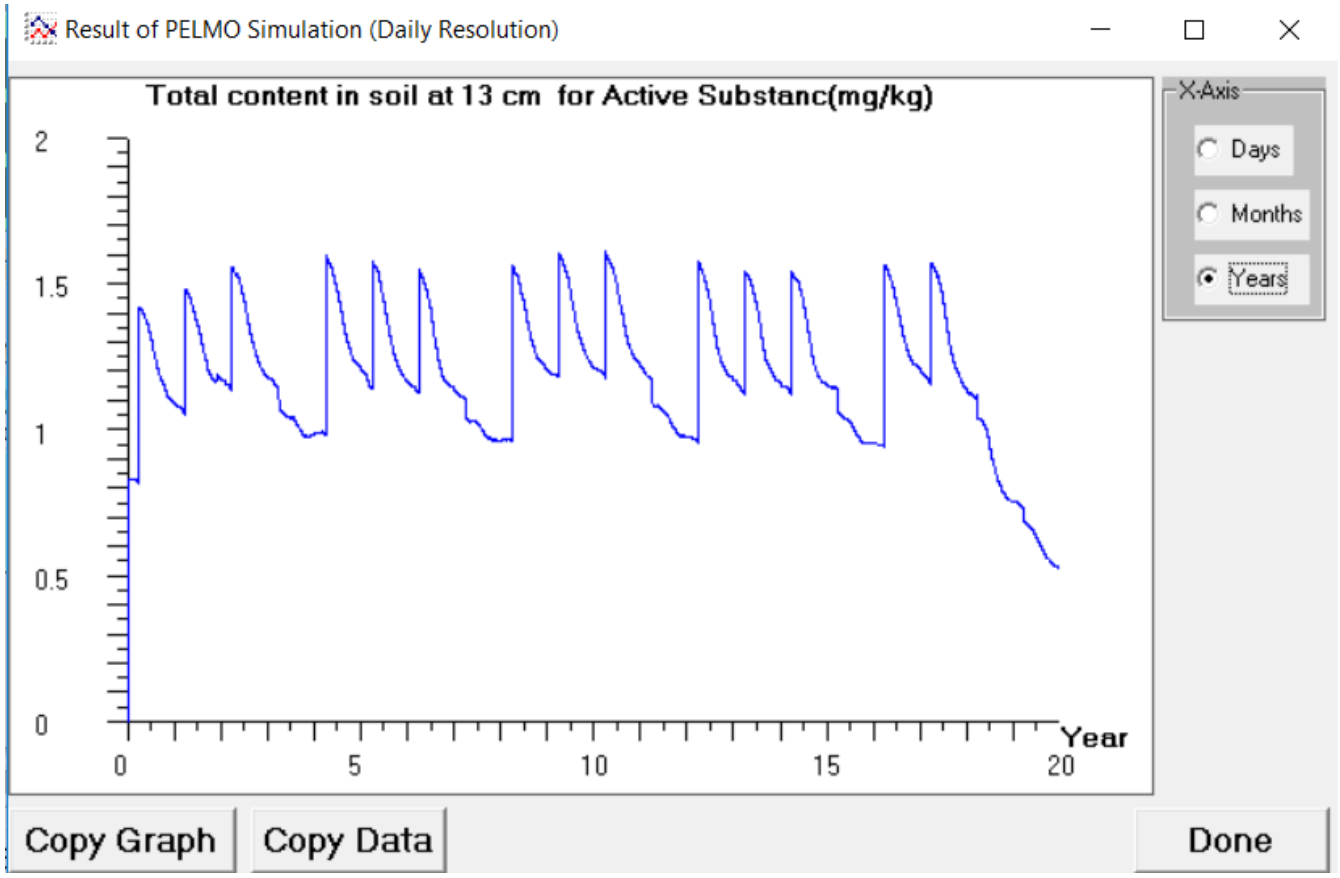
Tier 3A with PELMO: Placing of granules at a certain soil depth

Case 2 : placing at certain soil depth

Results

Table of actual and time weighted average concentrations in soil

```
         Tier 3A simulation:

         *** FOCUS PELMO  6. 6. 1 *** (PELMO 5.0)
         Compound: 04_2_Maize_1x_PlacedAt10cm_A_CTC
         Soil:     Medium (5.51% 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): 10



       Substance:      P (PesticideA)

       TWA(d)          PEC(mg/kg)      Begin TWA(d)
          0               3.6242820    1 April 43
          1               3.6236980    1 April 43
          2               3.6227450    1 April 43
          4               3.6223730    1 April 43
          7               3.6195869    1 April 43
         14               3.6107739    1 April 43
         21               3.6014895    1 April 43
         28               3.5917691    1 April 43
         42               3.5720223    1 April 43
         56               3.5550759    1 April 43
        100               3.4921157    1 April 43
Plateau (20 cm)           1.1212250    01 April 43

Conc. after 90 d          1.4177850    30 June 50
Conc. after 120 d         1.3162600    30 July 50
Conc. after 165 d         1.1968910    13 September 50
Conc. after 200 d         1.1481525    18 October 50
Conc. after 270 d         1.0816290    27 December 50
Conc. after 320 d         1.0591495    15 February 51
Conc. after 365 d         1.0347100    01 April 51
```



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