

June 5, 2019

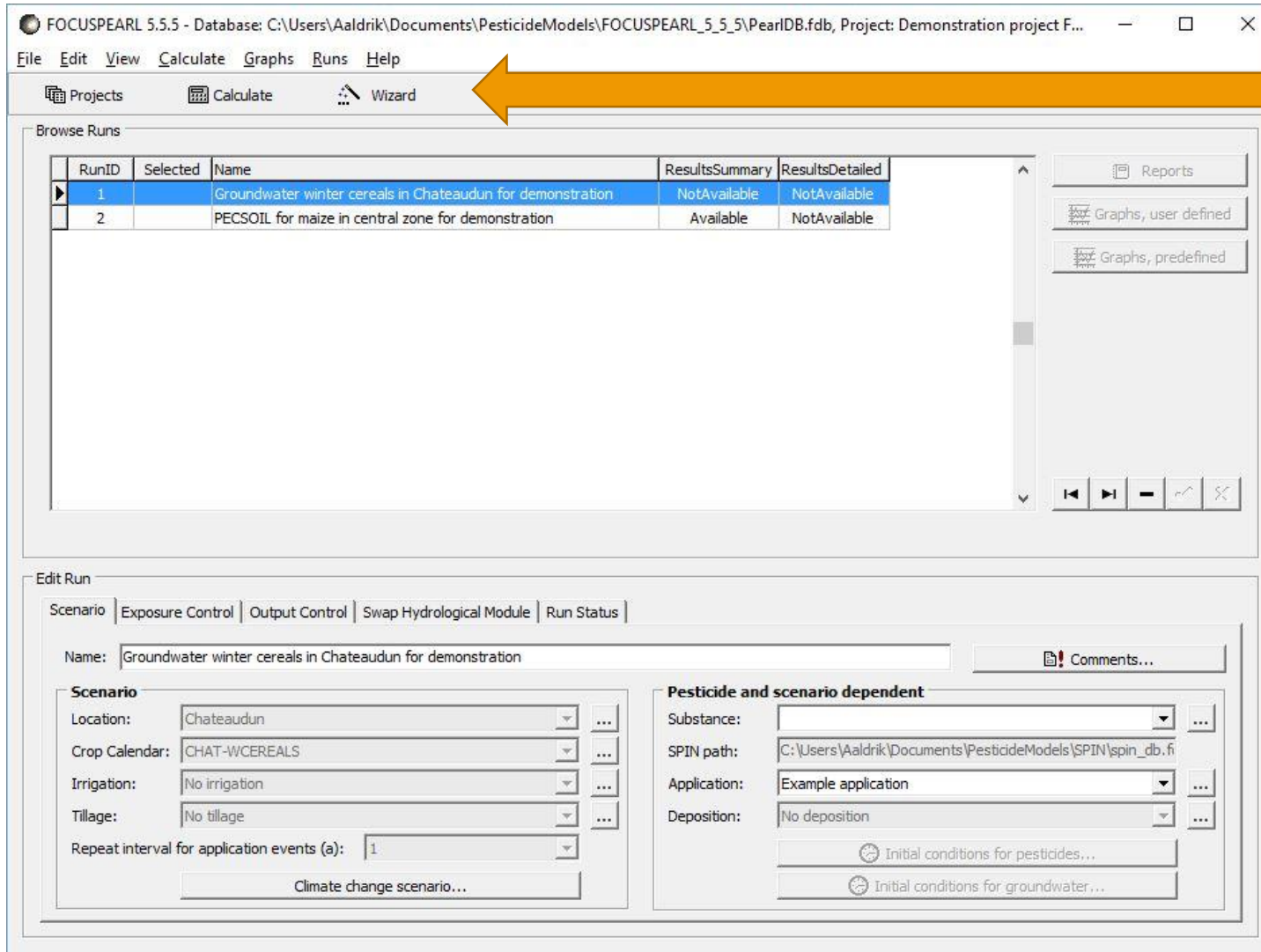
# The EFSA Guidance on PECs in soil: Using the PEARL Model

**EFSA info session 4/5 June 2019**

Aaldrik Tiktak

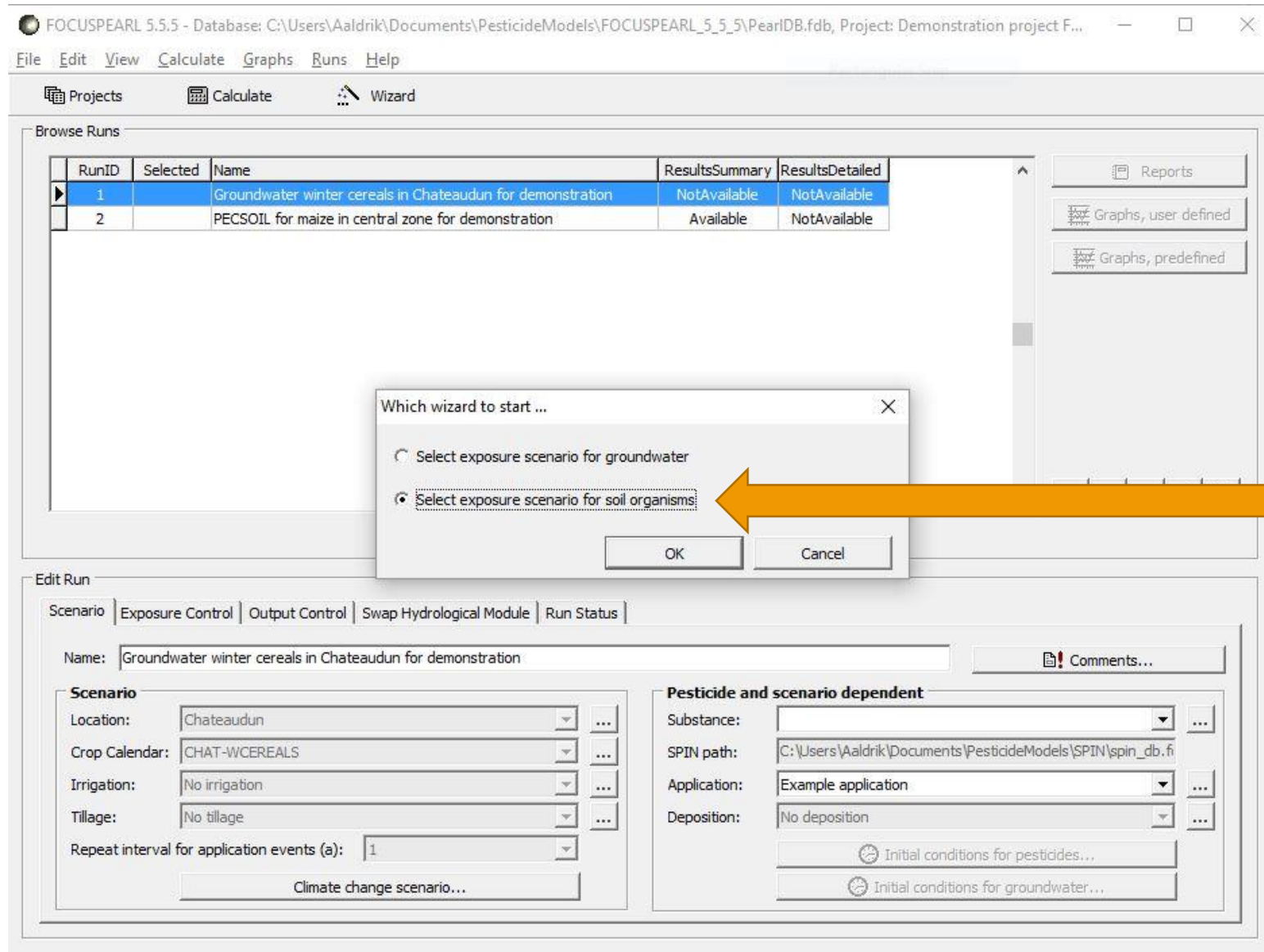
Trusted science for safe food

# Reading the PERSAM transfer files



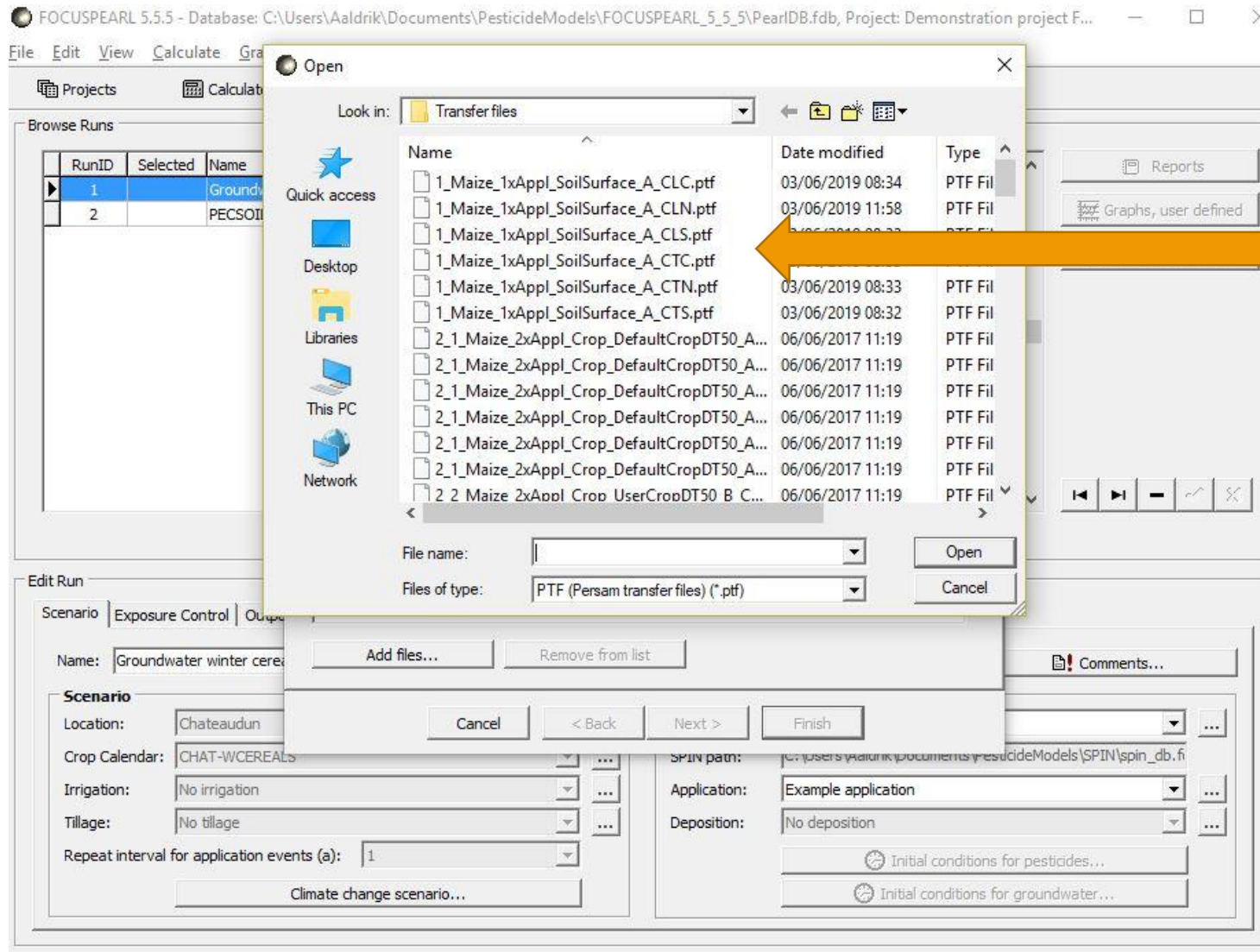
Open the wizard from the start screen

# Reading the PERSAM transfer files



Select the soil exposure scenarios

# Reading the PERSAM transfer files



Multiple transfer files  
can be selected by  
holding the SHIFT-key

When done select Next



# Select the application scheme

FOCUSPEARL 5.5.5 - Database: C:\Users\Aaldrik\Documents\PesticideModels\FOCUSPEARL\_5\_5\_5\PearlDB.fdb, Project: Demonstration project F...

File Edit View Calculate Graphs Runs Help

Projects Calculate Wizard

Browse Runs

RunID	Selected	Name	ResultsSummary	ResultsDetailed
1	<input checked="" type="checkbox"/>	Groundwater winter cereals in Chateaudun for demonstration	NotAvailable	NotAvailable
2	<input type="checkbox"/>	PECSOIL for demonstration	Available	NotAvailable

Wizard for Tier3B run creation...

Select type of application date

☒ Relative

Select type of event

☒ Emergence

☐ Harvest

Number of days before or after the event:

0

☐ Absolute

Date of first application:

<choose date>

Cancel < Back Next > Finish

Edit Run

Scenario Exposure Control Output

Name: Groundwater winter cereals

Scenario

Location: Chateaudun

Crop Calendar: CHAT-WCEREALS

Irrigation: No irrigation

Tillage: No tillage

Repeat interval for application events (a): 1

Climate change scenario...

SPIN path: C:\Users\Aaldrik\Documents\PesticideModels\SPIN\spin\_db.f

Application: Example application

Deposition: No deposition

Initial conditions for pesticides...

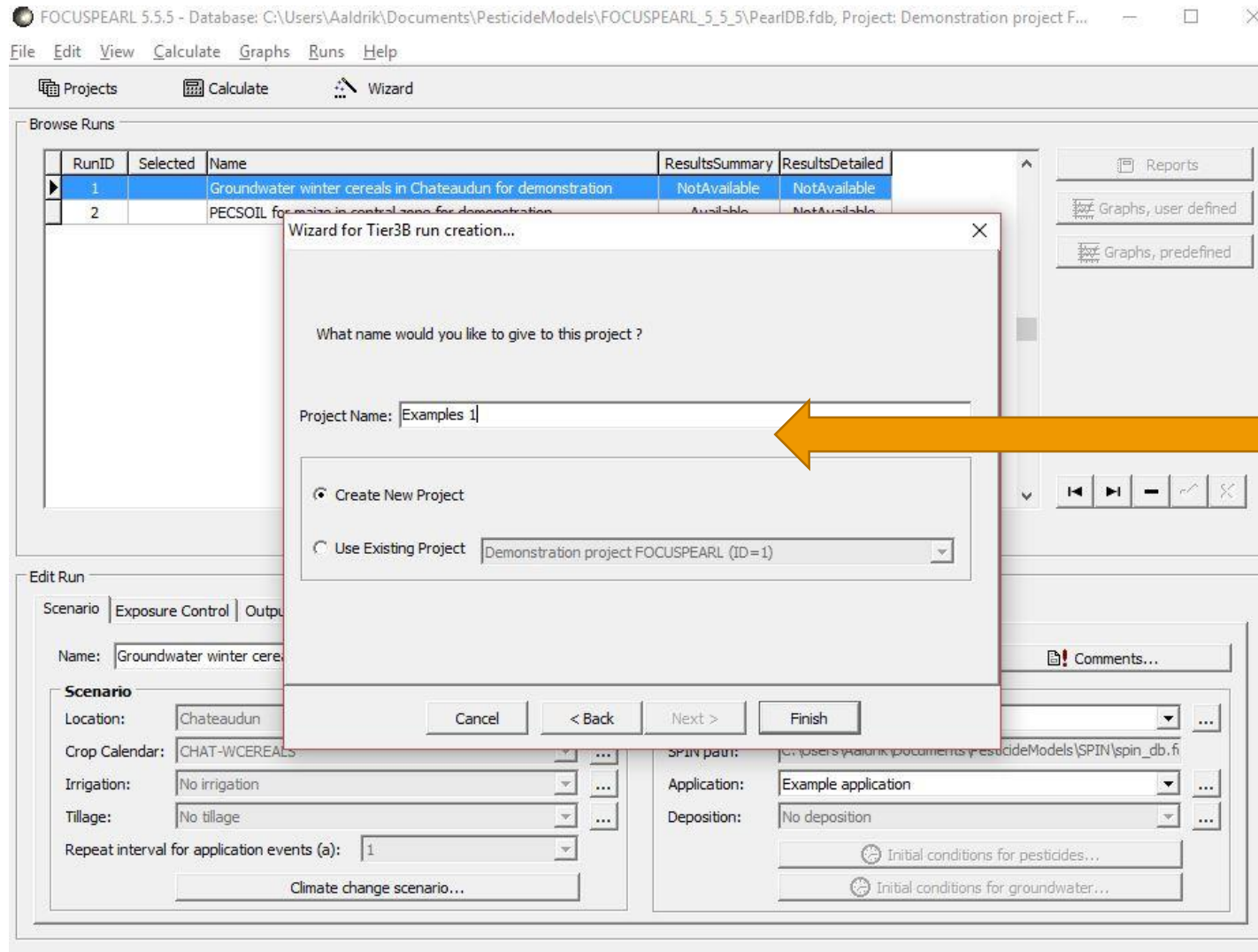
Initial conditions for groundwater...

Then select the application schedule

You can select absolute or relative application dates

When done select Next

# Add the runs to a project



Finally select the project to which you want to add the runs

Select Finish and PEARL will generate the runs

# Change the substance properties, if needed

FOCUSPEARL 5.5.5 - Database: C:\Users\Aaldrik\Documents\PesticideModels\FOCUSPEARL\_5\_5\_5\PearlDB.fdb, Project: Examples 1

File Edit View Calculate Graphs Runs Help

Projects Calculate Wizard

Browse Runs

RunID	Selected	Name	ResultsSummary	ResultsDetailed
8	Yes	Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	NotAvailable	NotAvailable
9	Yes	Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	NotAvailable	NotAvailable
10	Yes	Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	NotAvailable	NotAvailable
11	Yes	Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	NotAvailable	NotAvailable
12	Yes	Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	NotAvailable	NotAvailable
13	Yes	Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	NotAvailable	NotAvailable

Reports

Graphs, user defined

Graphs, predefined

Edit Run

Scenario Exposure Control Output Control Swap Hydrological Module Run Status

Name: Run generated from PERSAM file : 1\_Maize\_1xAppl\_SoilSurface\_A\_CTS.ptf (Substance PesticideA) Comments...

**Scenario**

Location: Southern Zone-CRS-HAMB (Tier3A) ...

Crop Calendar: HAMB-MAIZE ...

Irrigation: No irrigation ...

Tillage: 1 x 20cm, 30 days before emergence ...

Repeat interval for application events (a): 1 ...

Climate change scenario...

**Pesticide and scenario dependent**

Substance: PesticideA\_15 (Persam substance PesticideA\_15) ...

SPIN path: C:\Users\Aaldrik\Documents\PesticideModels\SPIN\spin\_db.fi ...

Application: Scheme generated from PERSAM file : 1\_Maize\_1xAppl ...

Deposition: No deposition ...

Initial conditions for pesticides...

Initial conditions for groundwater...

You will now see all the runs in the project

You can change substance properties if needed

# Editing the substance properties

SPIN (Substances Plug IN) 3.3 - Data required for PEARL for FOCUSPEARL, compartments All

File Help

### Browse Substances

Locked	SubstanceCode /	Name	CreationDate	LastModified
	PesticideA_1	Persam substance PesticideA_1	03/06/2019 08:36:08	03/06/2019 08:36:08
	PesticideA_10	Persam substance PesticideA_10	03/06/2019 12:01:52	03/06/2019 12:01:52
	PesticideA_11	Persam substance PesticideA_11	03/06/2019 12:01:52	03/06/2019 12:01:52
	PesticideA_12	Persam substance PesticideA_12	03/06/2019 12:01:52	03/06/2019 12:01:52
	PesticideA_13	Persam substance PesticideA_13	03/06/2019 12:01:52	03/06/2019 12:01:52
	PesticideA_14	Persam substance PesticideA_14	03/06/2019 12:01:52	03/06/2019 12:01:52
	PesticideA_15	Persam substance PesticideA_15	03/06/2019 12:01:53	03/06/2019 12:01:53
	PesticideA_2	Persam substance PesticideA_2	03/06/2019 08:36:08	03/06/2019 08:36:08
	PesticideA_3	Persam substance PesticideA_3	03/06/2019 08:36:08	03/06/2019 08:36:08
	PesticideA_4	Persam substance PesticideA_4	03/06/2019 08:36:08	03/06/2019 08:36:08
	PesticideA_5	Persam substance PesticideA_5	03/06/2019 08:40:51	03/06/2019 08:40:51
	PesticideA_6	Persam substance PesticideA_6	03/06/2019 08:40:51	03/06/2019 08:40:51
	PesticideA_7	Persam substance PesticideA_7	03/06/2019 08:40:51	03/06/2019 08:40:51
	PesticideA_8	Persam substance PesticideA_8	03/06/2019 08:40:52	03/06/2019 08:40:52

### Edit Substance

General | Sorption | Transformation | Crop processes

#### Canopy

Wash-off factor (m-1):

Canopy process option:

**Lumped**

Half-life on crop canopy (d):

#### Plant root

Coefficient for uptake by plant (TSCF) (-):

After opening the substance screen you see all the substances. Be careful to edit the substance in your run



# E.g. – how to change the wash-off factor

SPIN (Substances Plug IN) 3.3 - Data required for PEARL for FOCUSPEARL, compartments All

File Help

### Browse Substances

Locked	SubstanceCode /	Name	CreationDate	LastModified
	PesticideA_1	Persam substance PesticideA_1	03/06/2019 08:36:08	03/06/2019 08:36:08
	PesticideA_10	Persam substance PesticideA_10	03/06/2019 12:01:52	03/06/2019 12:01:52
	PesticideA_11	Persam substance PesticideA_11	03/06/2019 12:01:52	03/06/2019 12:01:52
	PesticideA_12	Persam substance PesticideA_12	03/06/2019 12:01:52	03/06/2019 12:01:52
	PesticideA_13	Persam substance PesticideA_13	03/06/2019 12:01:52	03/06/2019 12:01:52
	PesticideA_14	Persam substance PesticideA_14	03/06/2019 12:01:52	03/06/2019 12:01:52
	PesticideA_15	Persam substance PesticideA_15	03/06/2019 12:01:53	03/06/2019 12:01:53
	PesticideA_2	Persam substance PesticideA_2	03/06/2019 08:36:08	03/06/2019 08:36:08
	PesticideA_3	Persam substance PesticideA_3	03/06/2019 08:36:08	03/06/2019 08:36:08
	PesticideA_4	Persam substance PesticideA_4	03/06/2019 08:36:08	03/06/2019 08:36:08
	PesticideA_5	Persam substance PesticideA_5	03/06/2019 08:40:51	03/06/2019 08:40:51
	PesticideA_6	Persam substance PesticideA_6	03/06/2019 08:40:51	03/06/2019 08:40:51
	PesticideA_7	Persam substance PesticideA_7	03/06/2019 08:40:51	03/06/2019 08:40:51
	PesticideA_8	Persam substance PesticideA_8	03/06/2019 08:40:52	03/06/2019 08:40:52

Click this button if ready

### Edit Substance

General | Sorption | Transformation | Crop processes

**Canopy**

Wash-off factor (m-1):

Canopy process option:

**Lumped**

Half-life on crop canopy (d):

**Plant root**

Coefficient for uptake by plant (TSCF) (-):

Click this button if ready

Example: change the wash-off factor

# Creating graphs – what to do before the run

FOCUSPEARL 5.5.5 - Database: C:\Users\Aaldrik\Documents\PesticideModels\FOCUSPEARL\_5\_5\_5\PearlDB.fdb, Project: Examples 1

File Edit View Calculate Graphs Runs Help

Projects Calculate Wizard

Browse Runs

RunID	Selected	Name	ResultsSummary	ResultsDetailed
8		Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	Available	NotAvailable
9		Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	Available	NotAvailable
10		Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	Available	NotAvailable
11		Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	Available	NotAvailable
12		Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	Available	NotAvailable
13	<input checked="" type="checkbox"/>	Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	Available	Available

Reports

☒ Graphs, user defined

☒ Graphs, predefined

Click here to control the output

Edit Run

Scenario Exposure Control Output Control Hydrological Module Run Status

**General**

Format of time column in output file: Number of days since start of simulation

Print method: Month Print timestep (d): 30

Depth of leaching target layer (m): 1 Bottom: 0.05

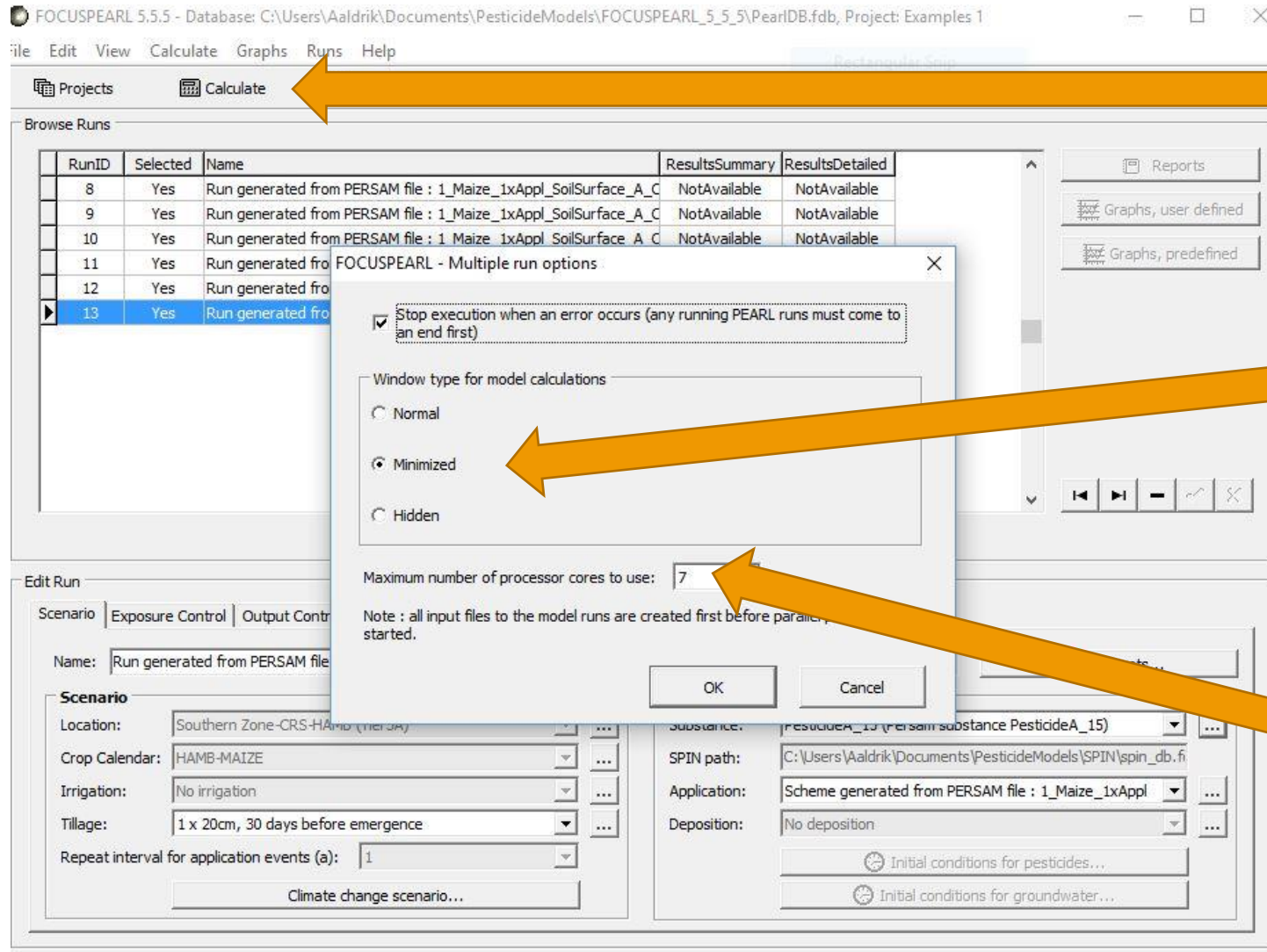
Ecotoxicological Averaging Depth (m) Top: 0

Detailed output: ☒

Detailed output options ...

And check this box

# Now you're ready to run...

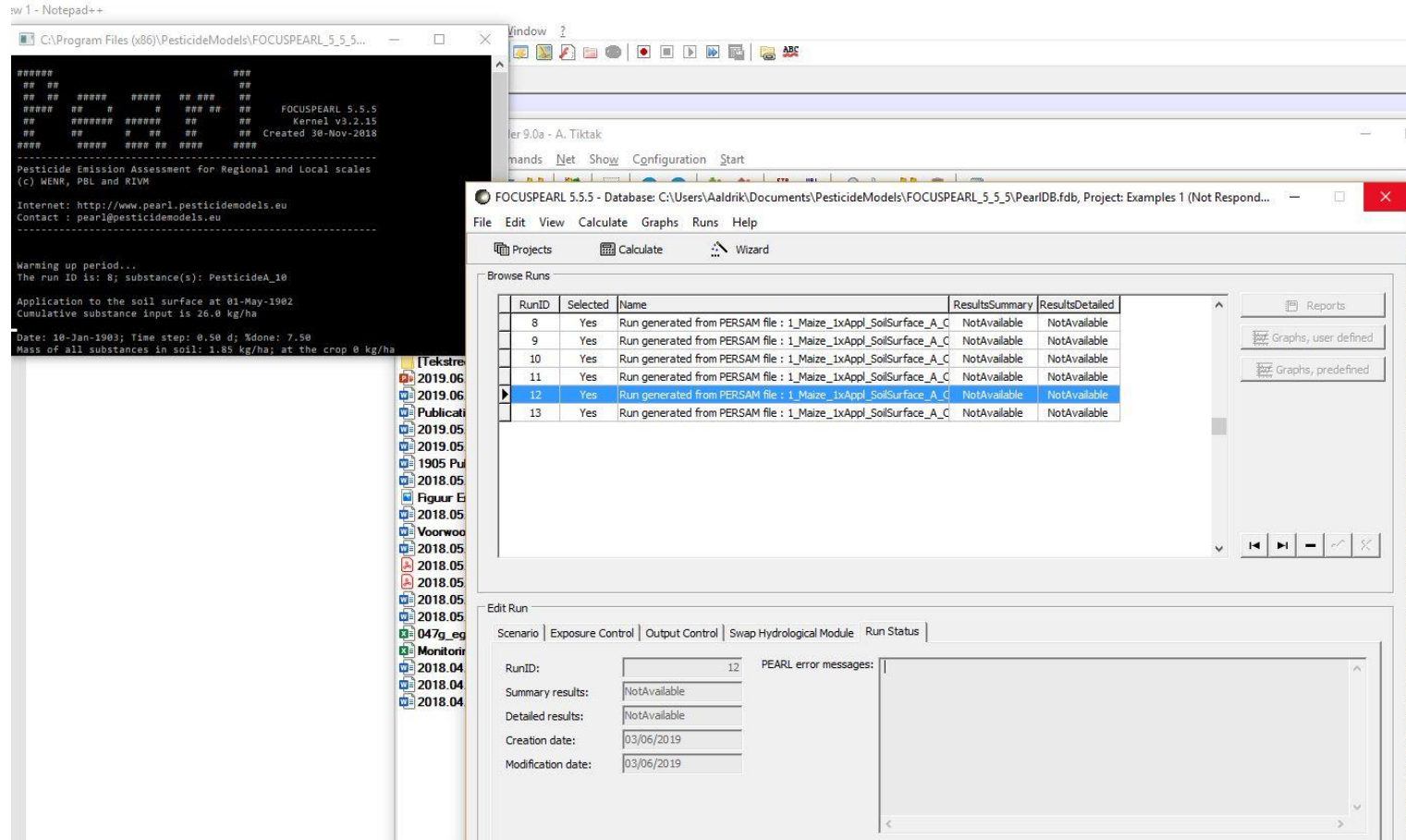


Click Calculate to run PEARL

With this you can control if you want to see progress of the runs

PEARL will use as many processors in your computer as possible

# ... and enjoy your coffee



Now wait.....



# Click report to see the results

FOCUSPEARL 5.5.5 - Database: C:\Users\Aaldrik\Documents\PesticideModels\FOCUSPEARL\_5\_5\_5\PearlDB.fdb, Project: Examples 1

File Edit View Calculate Graphs Runs Help

Projects Calculate Wizard

Browse Runs

RunID	Selected	Name	ResultsSummary	ResultsDetailed
8		Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	Available	NotAvailable
9		Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	Available	NotAvailable
10		Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	Available	NotAvailable
11		Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	Available	NotAvailable
12		Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	Available	NotAvailable
13		Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	Available	NotAvailable

Report

Graphs, user defined

Graphs, predefined

Edit Run

Scenario Exposure Control Output Control Swap Hydrological Module Run Status

RunID: 13

Summary results: Available

Detailed results: NotAvailable

Creation date: 03/06/2019

Modification date: 03/06/2019

PEARL error messages:

Click report to see the results

# Results are in the Soil Report

```
* PEARL REPORT: Soil
* -----
*
* Start date      : 01-Jan-1901
* End date        : 31-Dec-1927
* Thickness of evaluation layer 0.05 (m)
*
* This assessment is only valid for substance: PesticideA
*
* Annual application to the soil surface at 05-May; dosage = 1.0000 kg.ha-1
*
* Summary for substance PesticideA_15
* Molar mass (g.mol-1) : 300.0
* Saturated vapour pressure (Pa) : 0.100E-07; measured at (C) 20.0
* Solubility in water (mg.L-1) : 0.100 ; measured at (C) 20.0
* Half-life (d) in soil : 250.0; measured at (C) 20.0
* Kom (coef. for sorption on soil organic matter) (L.kg-1) : 1000.0
* KF (overall sorption coefficient of the soil target layer) (L.kg-1) : 39.9
* Freundlich exponent (-) : 0.90
* Plant uptake factor (-) : 0.00
*
* Pore water concentration (mg/L)
PesticideA_15 TWA_ConLiq_0 0.031620 at 05-May-1912
PesticideA_15 TWA_ConLiq_7 0.031401 at 05-May-1912
PesticideA_15 TWA_ConLiq_14 0.031253 at 05-May-1912
PesticideA_15 TWA_ConLiq_21 0.030819 at 05-May-1912
PesticideA_15 TWA_ConLiq_28 0.030301 at 05-May-1912
PesticideA_15 TWA_ConLiq_56 0.028217 at 05-May-1912
PesticideA_15 TWA_ConLiq_100 0.025899 at 05-May-1912
*
* Concentration in total soil (mg/kg)
PesticideA_15 TWA_CntSys_0 2.610677 at 05-May-1912
PesticideA_15 TWA_CntSys_7 2.603787 at 05-May-1912
PesticideA_15 TWA_CntSys_14 2.597109 at 05-May-1912
PesticideA_15 TWA_CntSys_21 2.590690 at 05-May-1912
PesticideA_15 TWA_CntSys_28 2.584089 at 05-May-1912
PesticideA_15 TWA_CntSys_56 2.533628 at 05-May-1912
PesticideA_15 TWA_CntSys_100 2.423588 at 05-May-1912
```

And here are the results

# PEARL can read the PERSAM transfer files

FOCUSPEARL 5.5.5 - Database: C:\Users\Aaldrik\Documents\PesticideModels\FOCUSPEARL\_5\_5\_5\PearlDB.fdb, Project: Examples 1

File Edit View Calculate Graphs Runs Help

Projects Calculate Wizard

Browse Runs

RunID	Selected	Name	ResultsSummary	ResultsDetailed
8		Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	Available	NotAvailable
9		Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	Available	NotAvailable
10		Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	Available	NotAvailable
11		Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	Available	NotAvailable
12		Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	Available	NotAvailable
13	<input checked="" type="checkbox"/>	Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	Available	Available

Reports

Graphs, user defined

Graphs, predefined

Edit Run

Scenario Exposure Control Output Control Hydrological Module Run Status

**General**

Format of time column in output file: Number of days since start of simulation

Print method: Month Print timestep (d): 30

Depth of leaching target layer (m): 1 Bottom: 0.05

Ecotoxicological Averaging Depth (m) Top: 0

Detailed output: ☒

Detailed output options ...

Click here to  
control the output

And check this  
box

# Make a graph of the total mass in soil

FOCUSPEARL 5.5.5 - Database: C:\Users\Aaldrik\Documents\PesticideModels\FOCUSPEARL\_5\_5\_5\PearlDB.fdb, Project: Examples 1

File Edit View Calculate Graphs Runs Help

Projects Calculate Wizard

Browse Runs

RunID	Selected	Name	ResultsSummary	ResultsDetailed
8		Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	Available	NotAvailable
9		Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	Available	NotAvailable
10		Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	Available	NotAvailable
11		Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	Available	NotAvailable
12		Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	Available	NotAvailable
13		Run generated from PERSAM file : 1_Maize_1xAppl_SoilSurface_A_C	Available	Available

Reports

Graphs, user defined

Graphs, predefined

Edit Run

Scenario Exposure Control Output Control Swap Hydrological Module Run Status

**General**

Format of time column in output file: Number of days since start of simulation

Print method: Month Print timestep (d): 30

Depth of leaching target layer (m): 1 Bottom: 0.05

Ecotoxicological Averaging Depth (m) Top: 0

Detailed output: ☒ Output cumulative: ☒

Detailed output options ...

Here you will find all kinds of graphs



# Select this one

FOCUSPEARL - User Defined Graphs

**Categories of variables available for graphs**

- ▶ Pearl Soil Balance
- Pearl Concentrations
- Pearl Crop Balance
- Pearl Fluxes
- Pearl General
- Pearl Vertical Profiles
- Swap Soil Fluxes
- Swap General

**Variables available for graphs in run**

Graph	Description Cumulative	HasDepth	IsCompoundVar	IsVertProfilevar
<input type="checkbox"/>	Areic mass of substance applied to the soil	No	No	No
<input type="checkbox"/>	Areic mass of substance in the equilibrium domain of the soil profile	No	Yes	No
<input type="checkbox"/>	Areic mass of substance in the equilibrium domain of the FOCUS layer	No	Yes	No
<input type="checkbox"/>	Areic numerical mass balance error	No	Yes	No
<input type="checkbox"/>	Areic mass of substance formed	No	Yes	No
<input type="checkbox"/>	Areic mass of substance in the non-equilibrium domain of the soil profile	No	Yes	No
<input type="checkbox"/>	Areic mass of substance in the non-equilibrium domain of the FOCUS layer	No	Yes	No
<input checked="" type="checkbox"/>	Areic mass of substance in the FOCUS layer	No	Yes	No
<input type="checkbox"/>	Areic mass of substance in the FOCUS layer	No	Yes	No
<input type="checkbox"/>	Areic mass of substance transformed	No	Yes	No

Substances:  
☒ PesticideA\_2

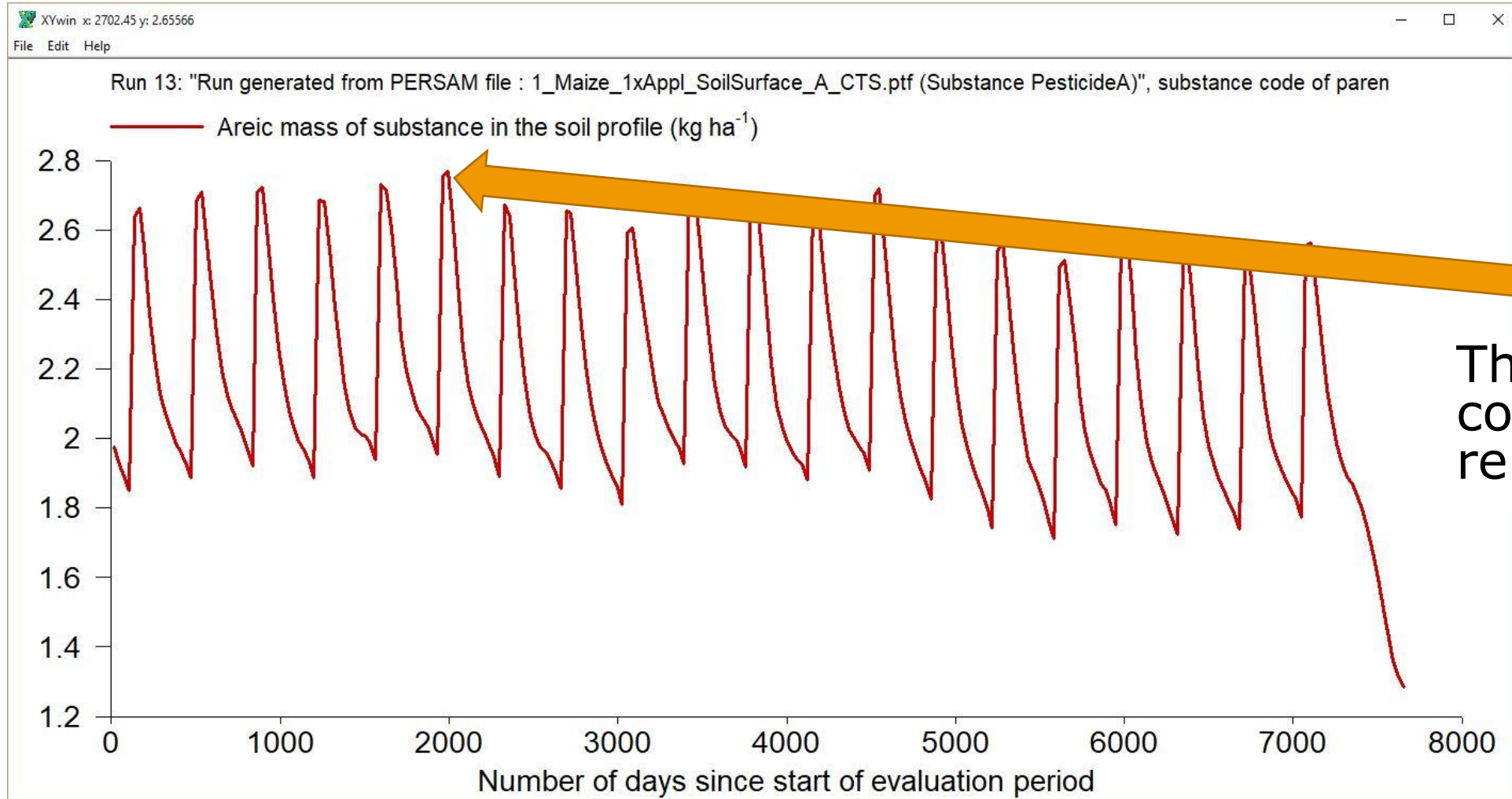
Export to file ... ☒ Graph Using Templ... ☒ Graph Using Templ...

Number of selected variables: 1

This is the graph  
of mass in the soil  
profile

And press this  
button

# This is all



This is the peak concentration reported