



June 5, 2019

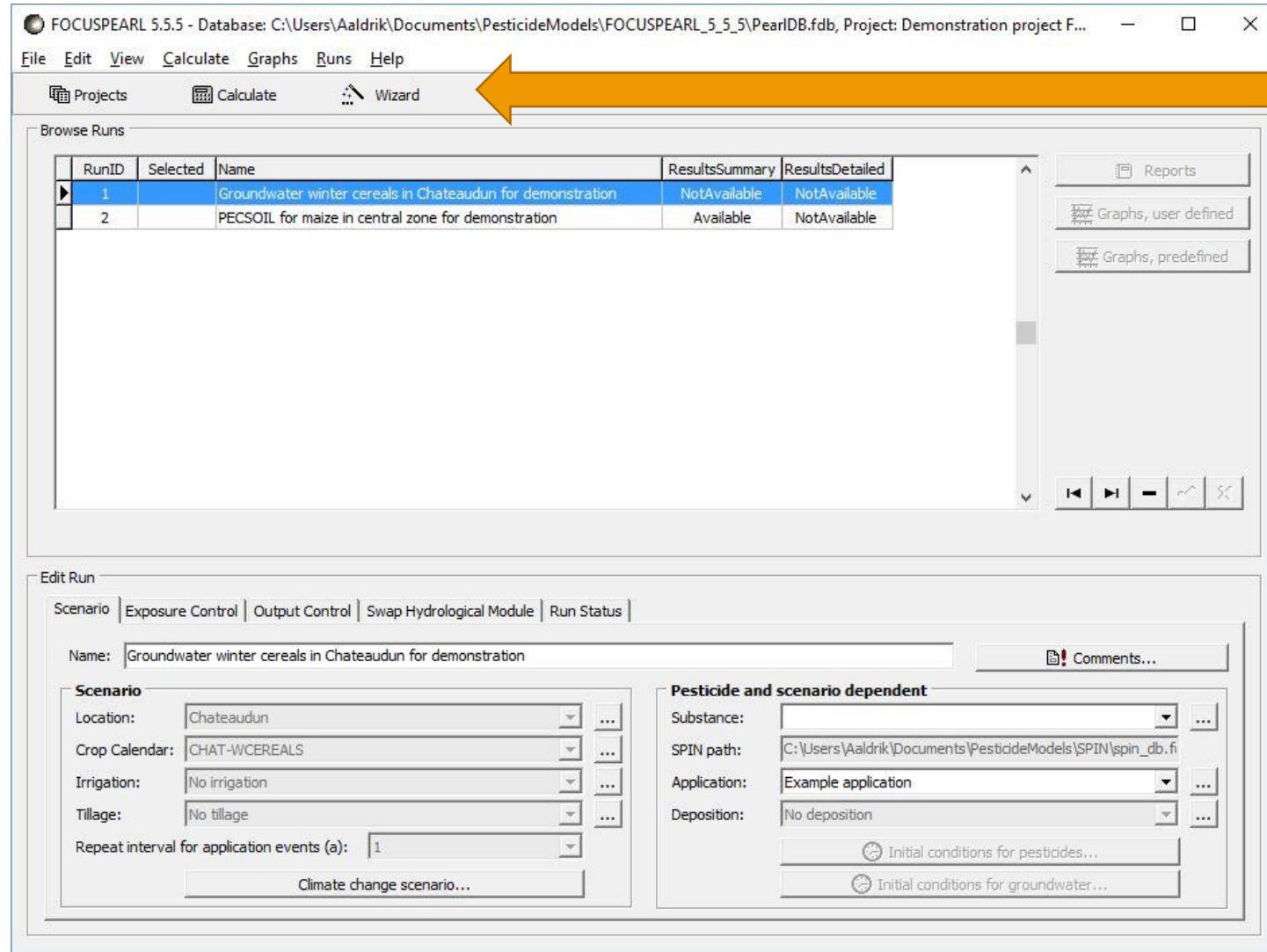
The EFSA Guidance on PECs in soil: Using the PEARL Model

EFSA info session 4/5 June 2019

Aaldrik Tiktak

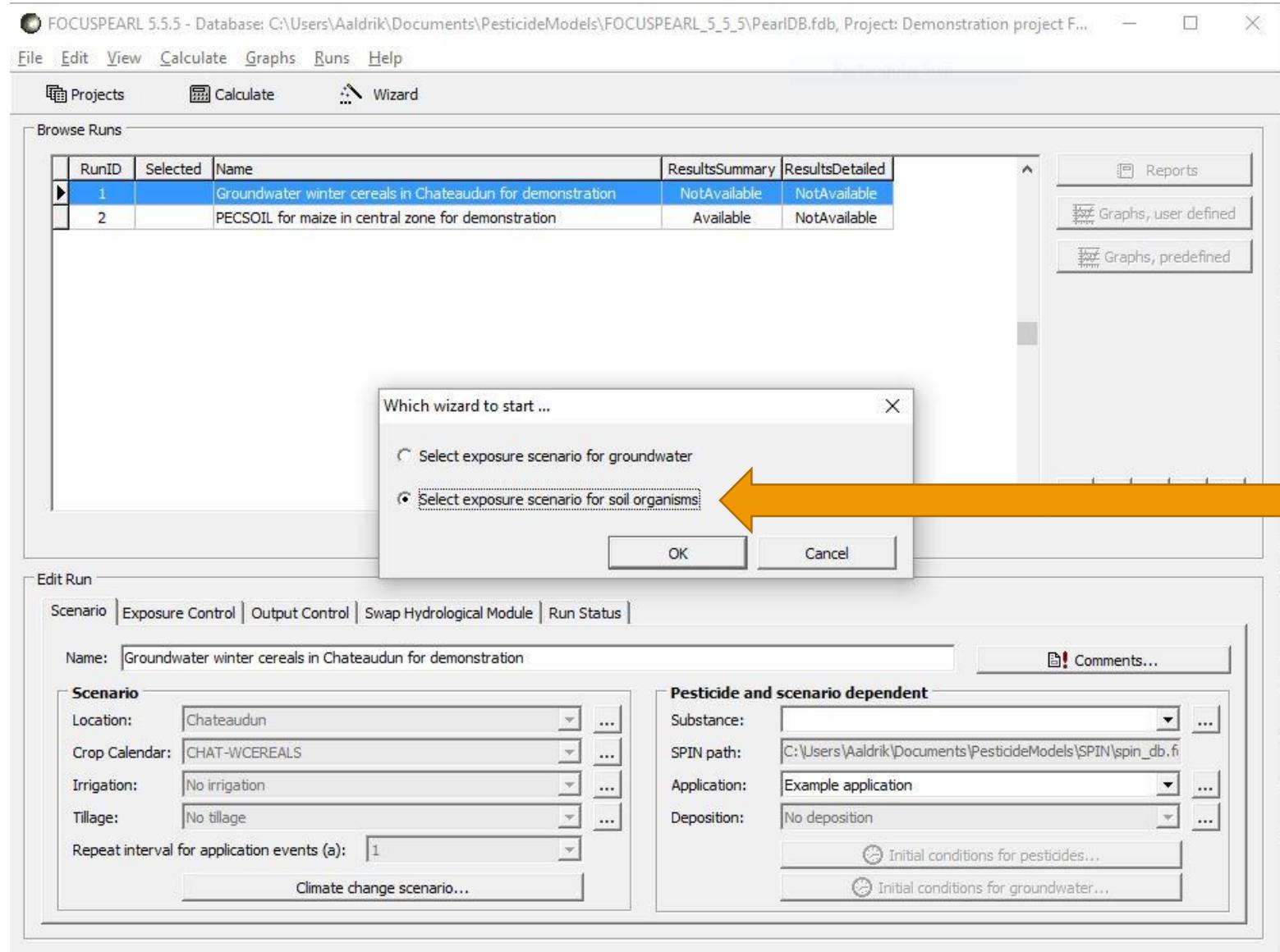
Trusted science for safe food

Reading the PERSAM transfer files



Open the wizard from the start screen

Reading the PERSAM transfer files



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		Groundwater winter cereals in Chateaudun for demonstration	NotAvailable	NotAvailable
2		PECSOIL for maize in central zone for demonstration	Available	NotAvailable

Reports

Graphs, user defined

Graphs, predefined

Which wizard to start ...

Select exposure scenario for groundwater

Select exposure scenario for soil organisms

OK Cancel

Edit Run

Scenario | Exposure Control | Output Control | Swap Hydrological Module | Run Status |

Name: Groundwater winter cereals in Chateaudun for demonstration

Comments...

Scenario

Location: Chateaudun

Crop Calendar: CHAT-WCEREALS

Irrigation: No irrigation

Tillage: No tillage

Repeat interval for application events (a): 1

Climate change scenario...

Pesticide and scenario dependent

Substance: [dropdown]

SPIN path: C:\Users\Aaldrik\Documents\PesticideModels\SPIN\spin_db.fi

Application: Example application

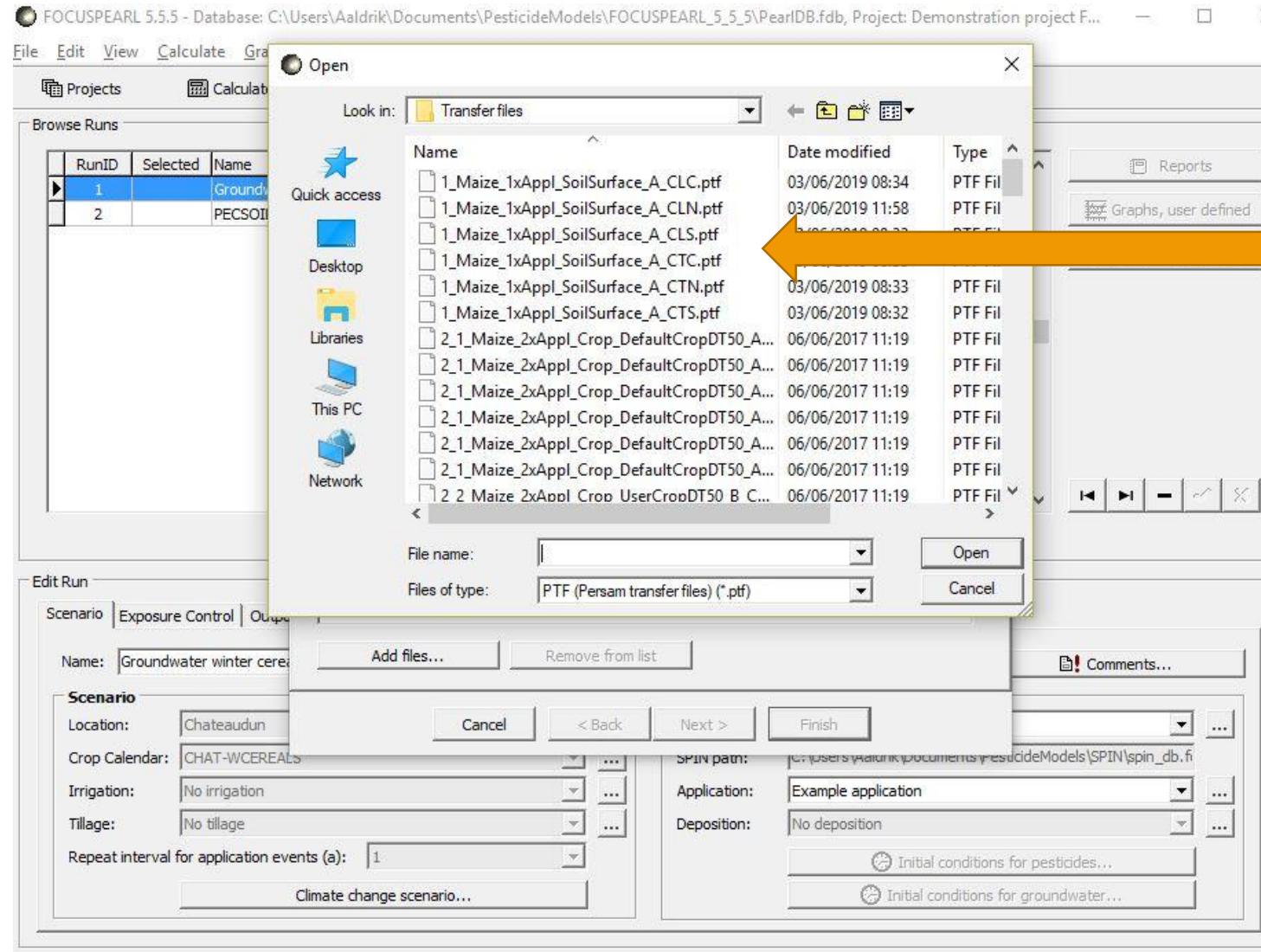
Deposition: No deposition

Initial conditions for pesticides...

Initial conditions for groundwater...

Select the soil exposure scenarios

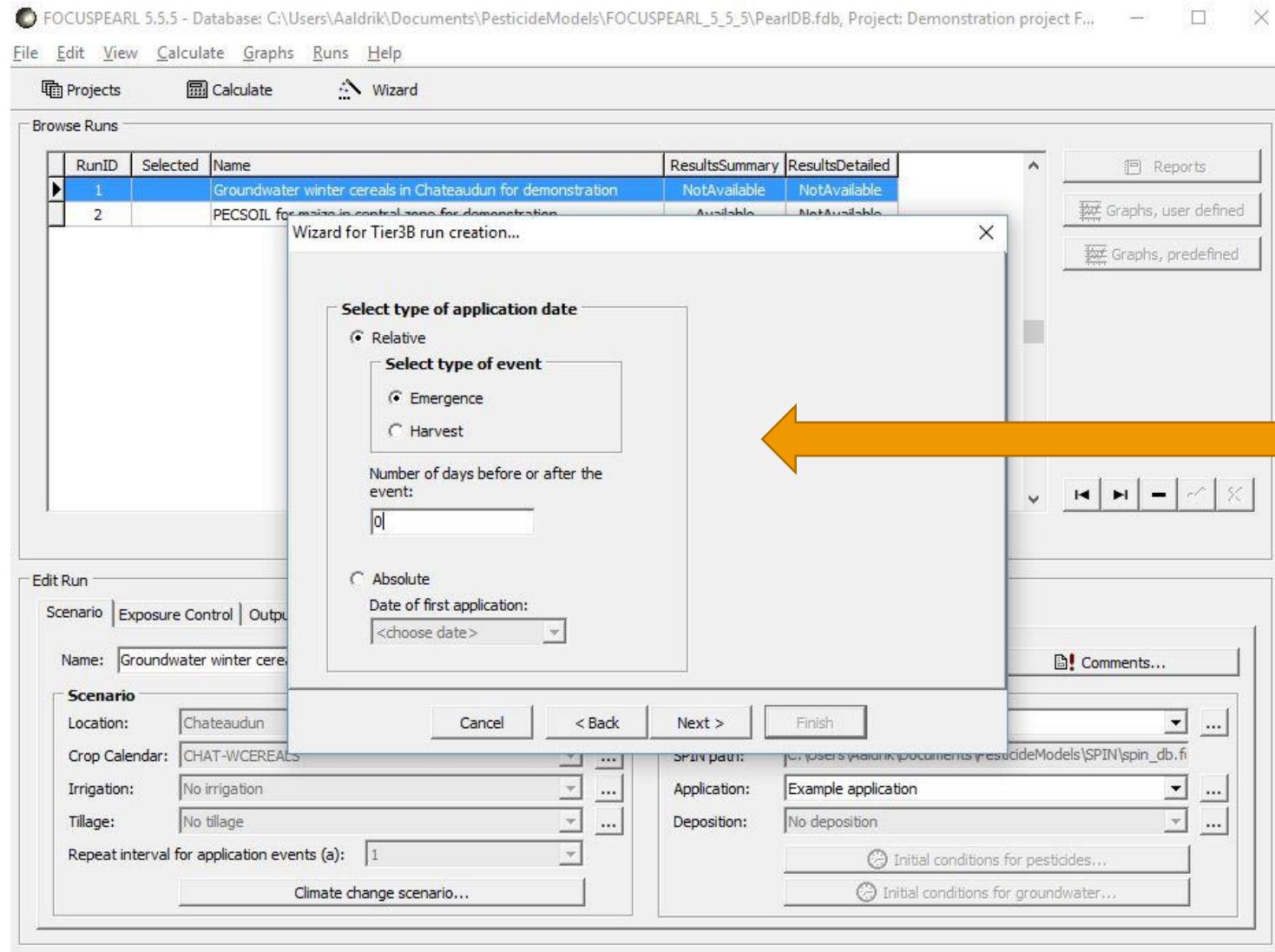
Reading the PERSAM transfer files



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

When done select Next

Select the application scheme

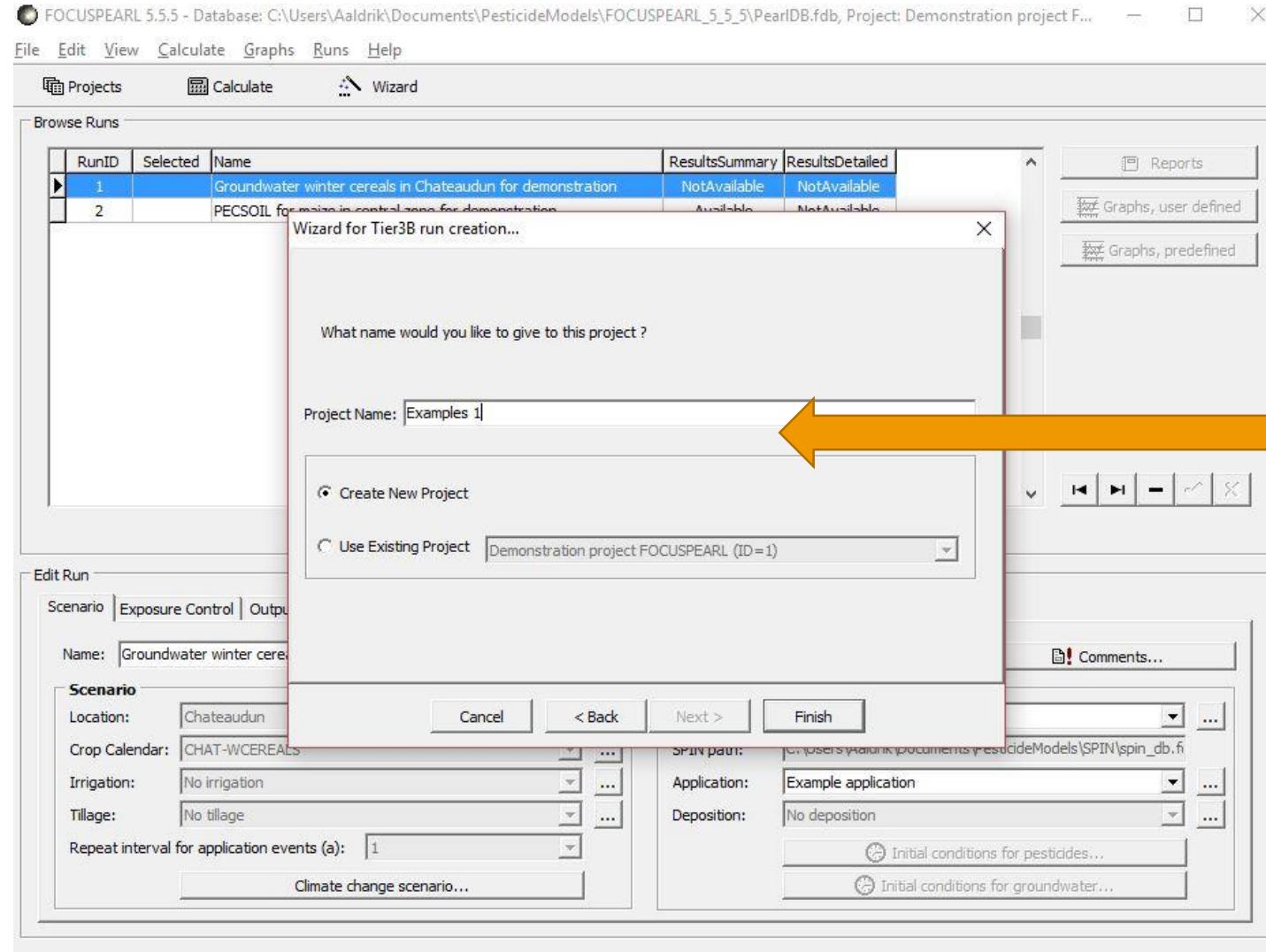


Then select the application schedule

You can select absolute or relative application dates

When done select Next

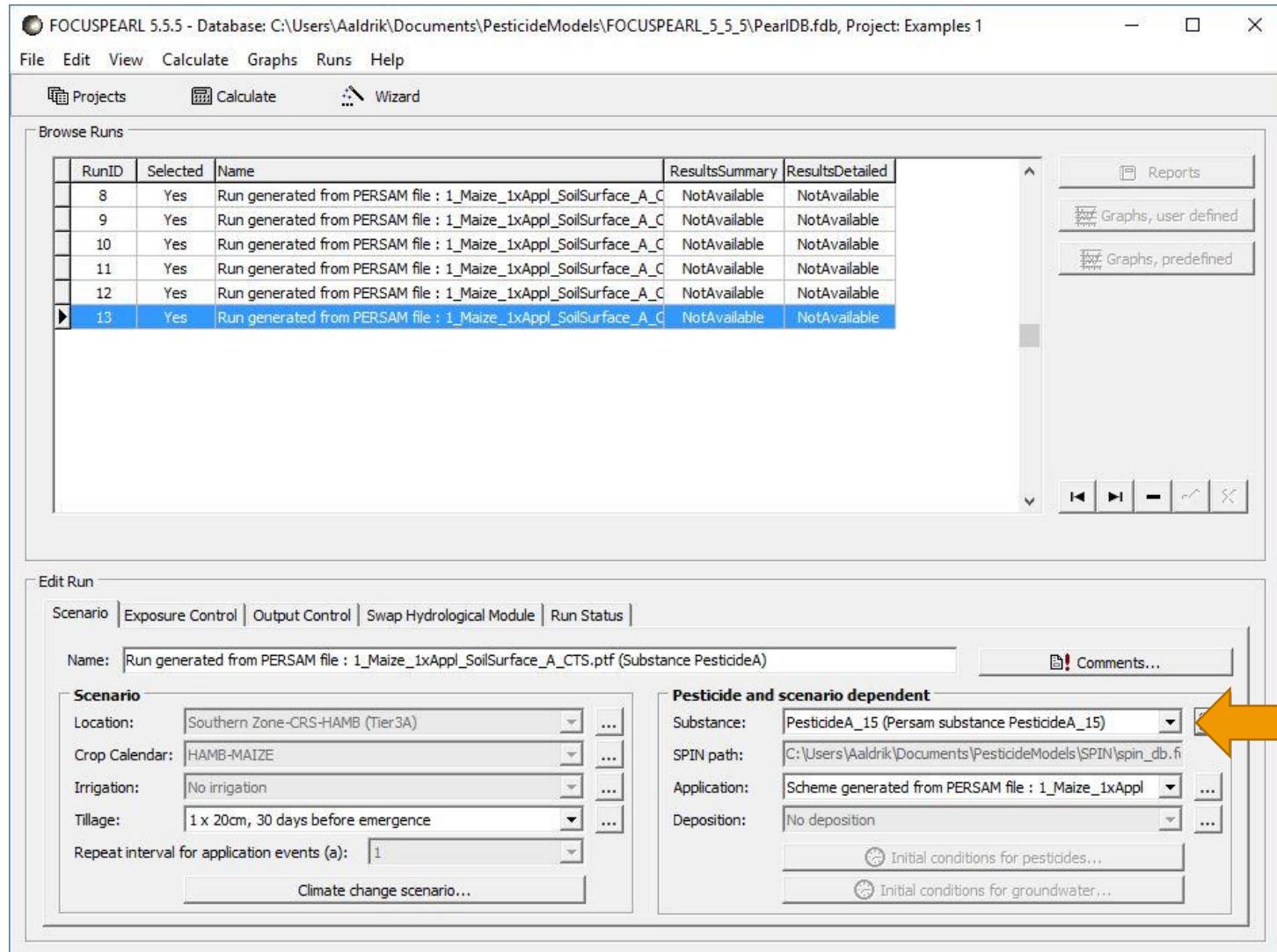
Add the runs to a project



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



The screenshot shows the FOCUSPEARL 5.5.5 software interface. The top menu bar includes File, Edit, View, Calculate, Graphs, Runs, and Help. The main window has tabs for Projects, Calculate, and Wizard. The 'Browse Runs' tab is active, displaying a table of runs with columns: RunID, Selected, Name, ResultsSummary, and ResultsDetailed. The 'Edit Run' tab is also visible, showing the 'Scenario' tab selected. It includes fields for Location (Southern Zone-CRS-HAMB (Tier3A)), Crop Calendar (HAMB-MAIZE), Irrigation (No irrigation), Tillage (1 x 20cm, 30 days before emergence), and a 'Repeat interval for application events (a)' field set to 1. The 'Edit Run' tab also contains a 'Comments...' button. The 'Pesticide and scenario dependent' section includes fields for 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), and Deposition (No deposition). A yellow arrow points from the text 'You can change substance properties if needed' to the 'Substance' dropdown in the 'Edit Run' section.

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

Edit Substance

General | Sorption | Transformation | Crop processes | **Crop processes**

Canopy

Wash-off factor (n-1): ⓘ

Canopy process option: ⓘ

Lumped

Half-life on crop canopy (d): ⓘ

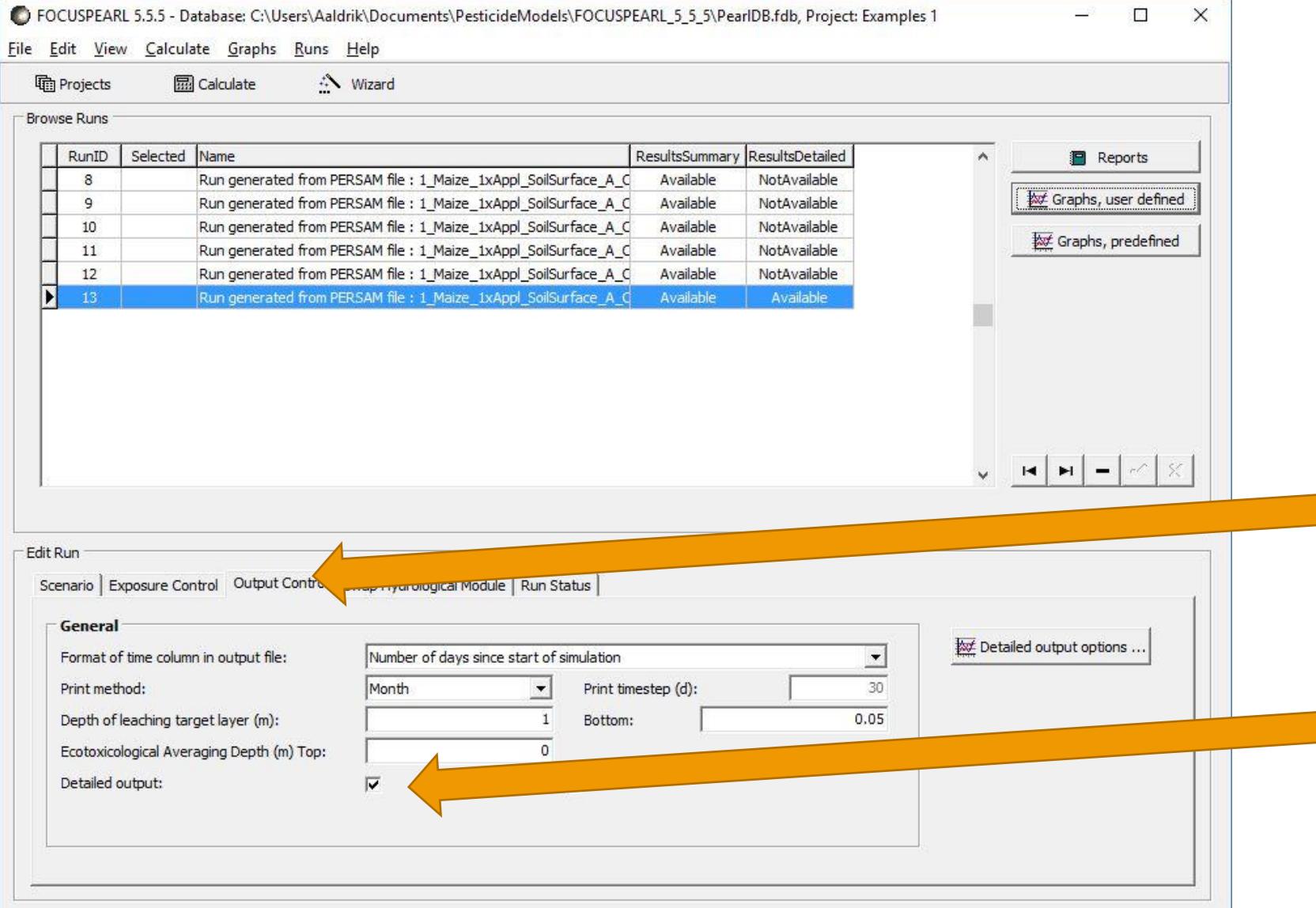
Plant root

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		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** | Crop 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

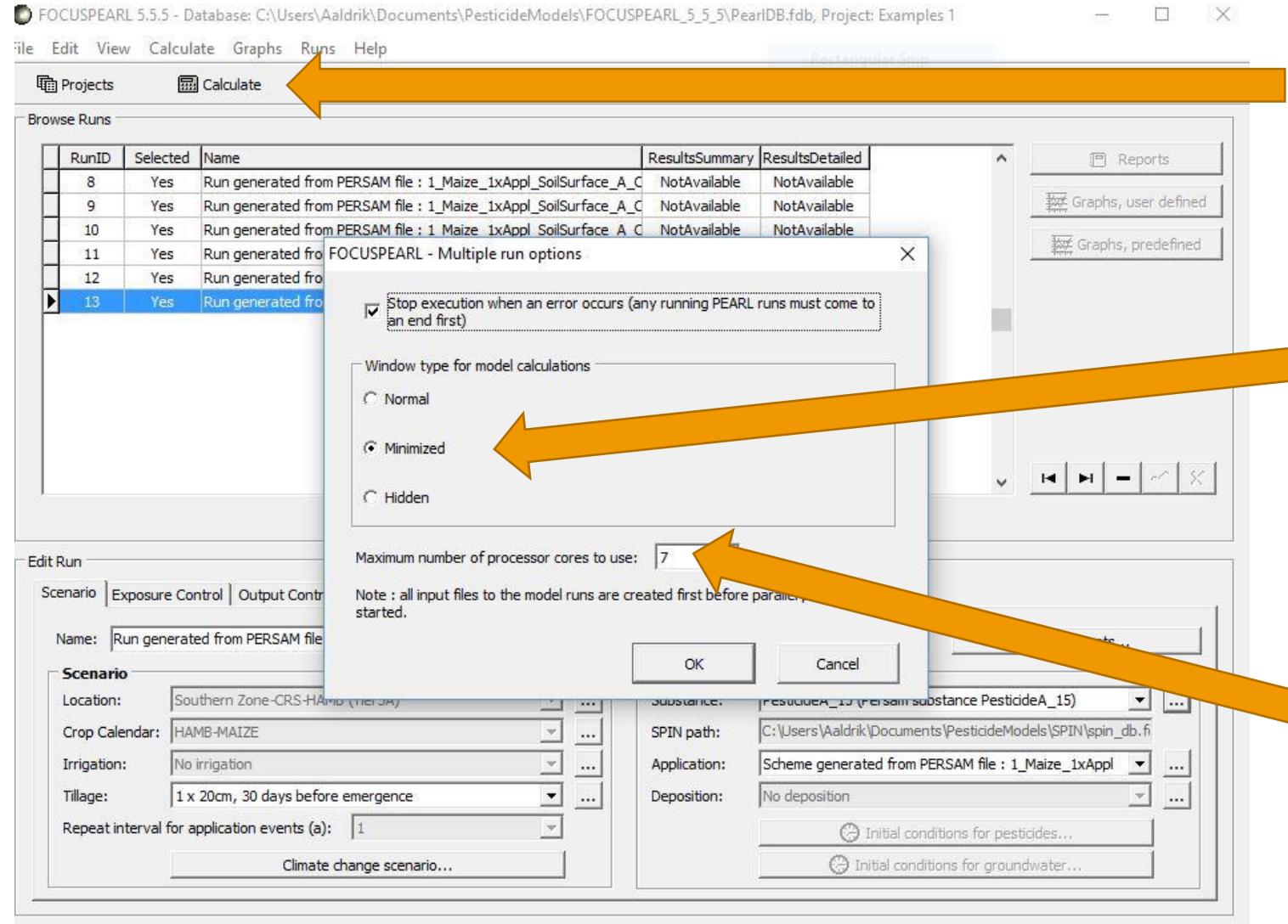
Ecotoxicological Averaging Depth (m) Top: 0

Detailed output: Detailed output options ...

Click here to control the output

And check this box

Now you're ready to run...

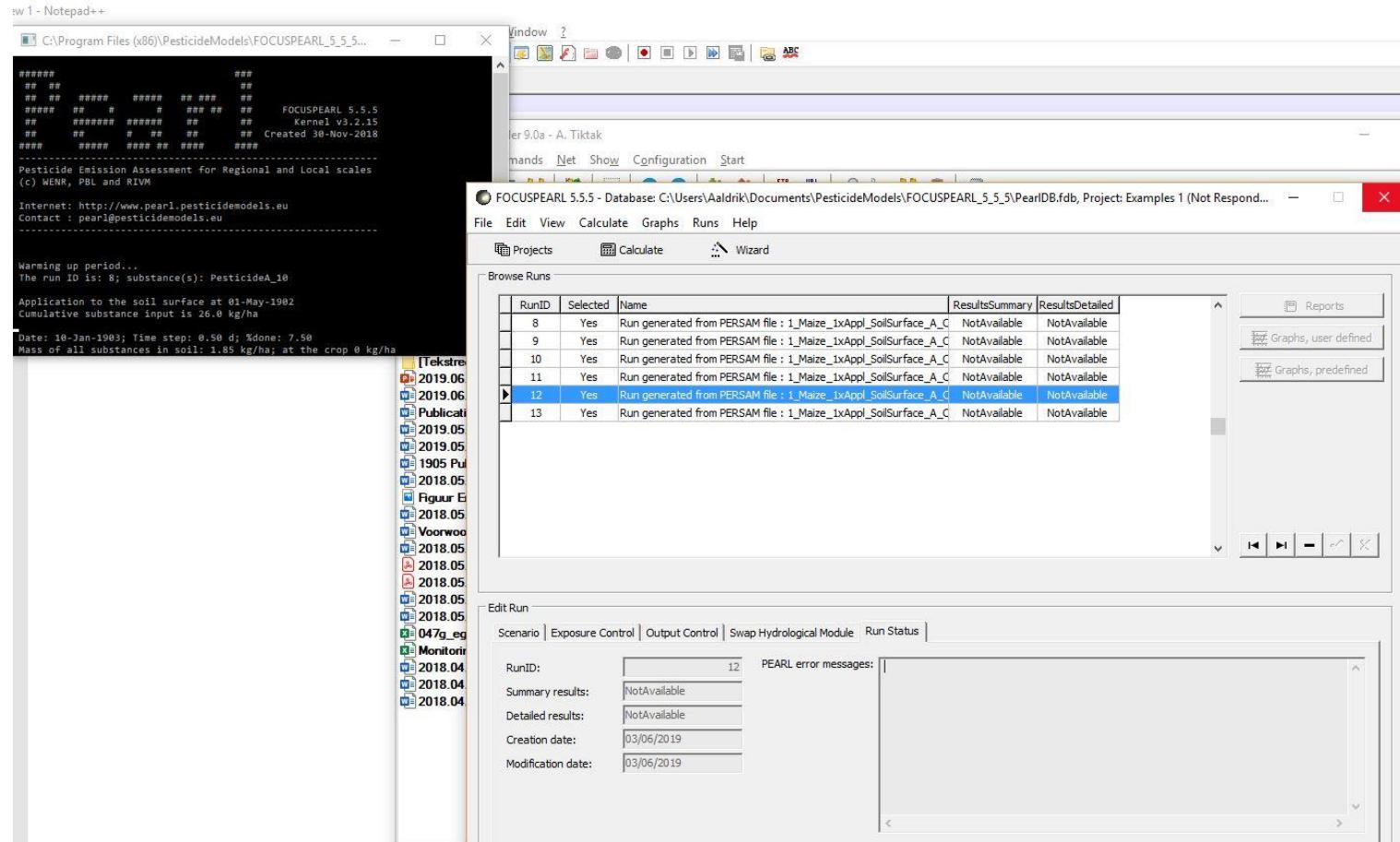


Click Calculate to run PEARL

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

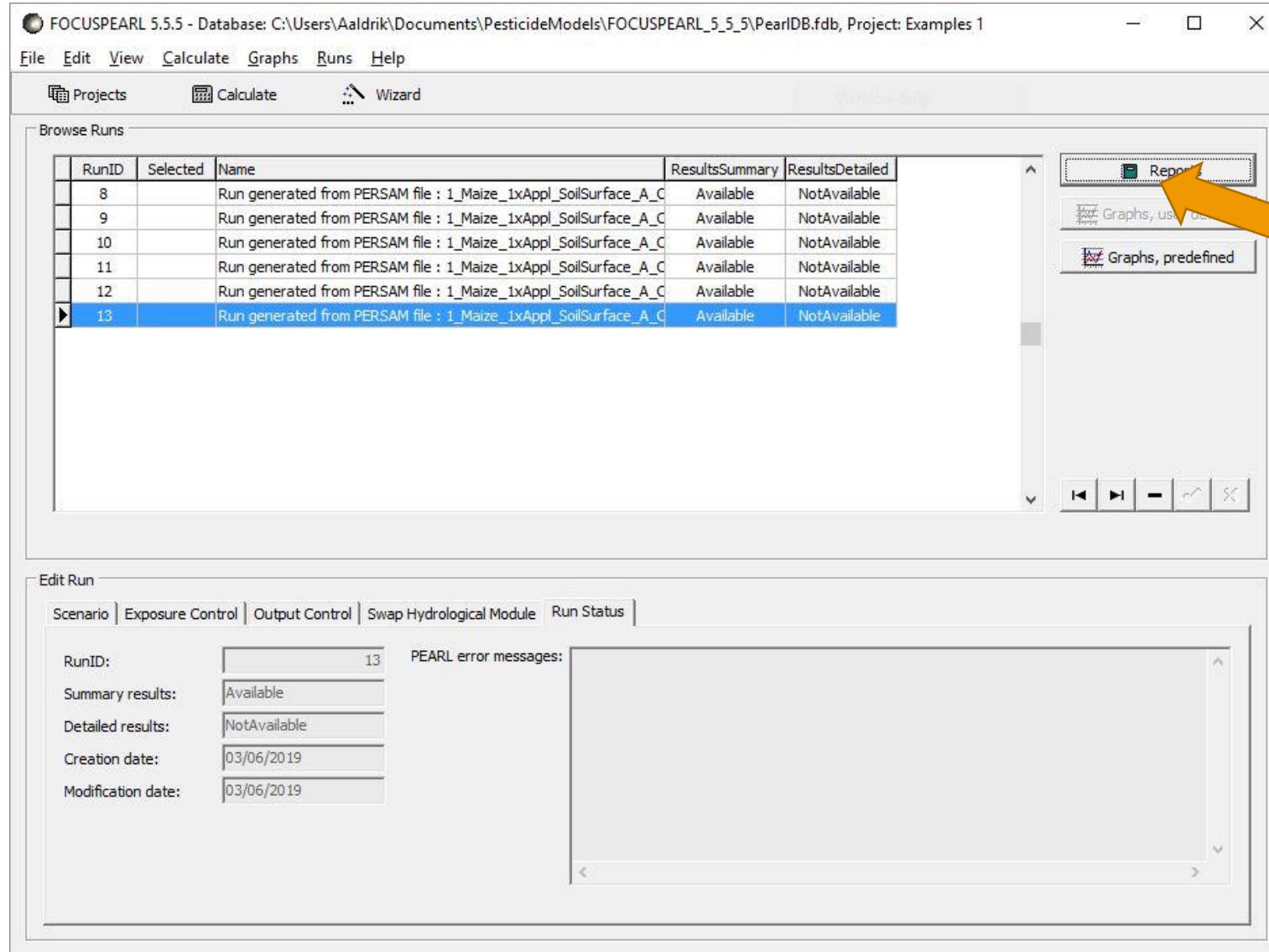
PEARL will use as many processors in your computer as possible

... 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

PEARL error messages:

Summary results: Available

Detailed results: NotAvailable

Creation date: 03/06/2019

Modification date: 03/06/2019

Click report to see the results

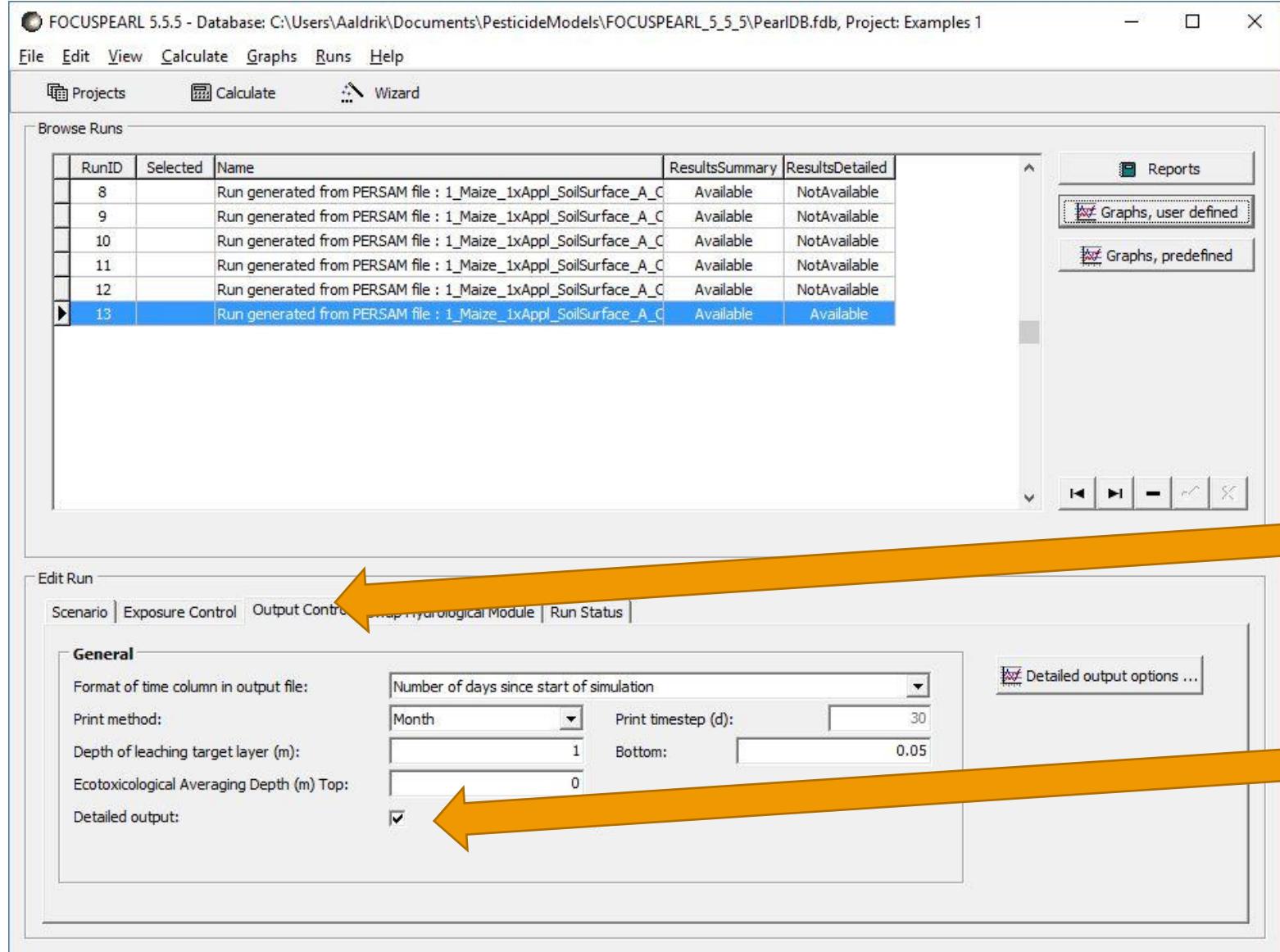
Results are in the Soil Report

```
* 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 (coeff. 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
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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** | Crop 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

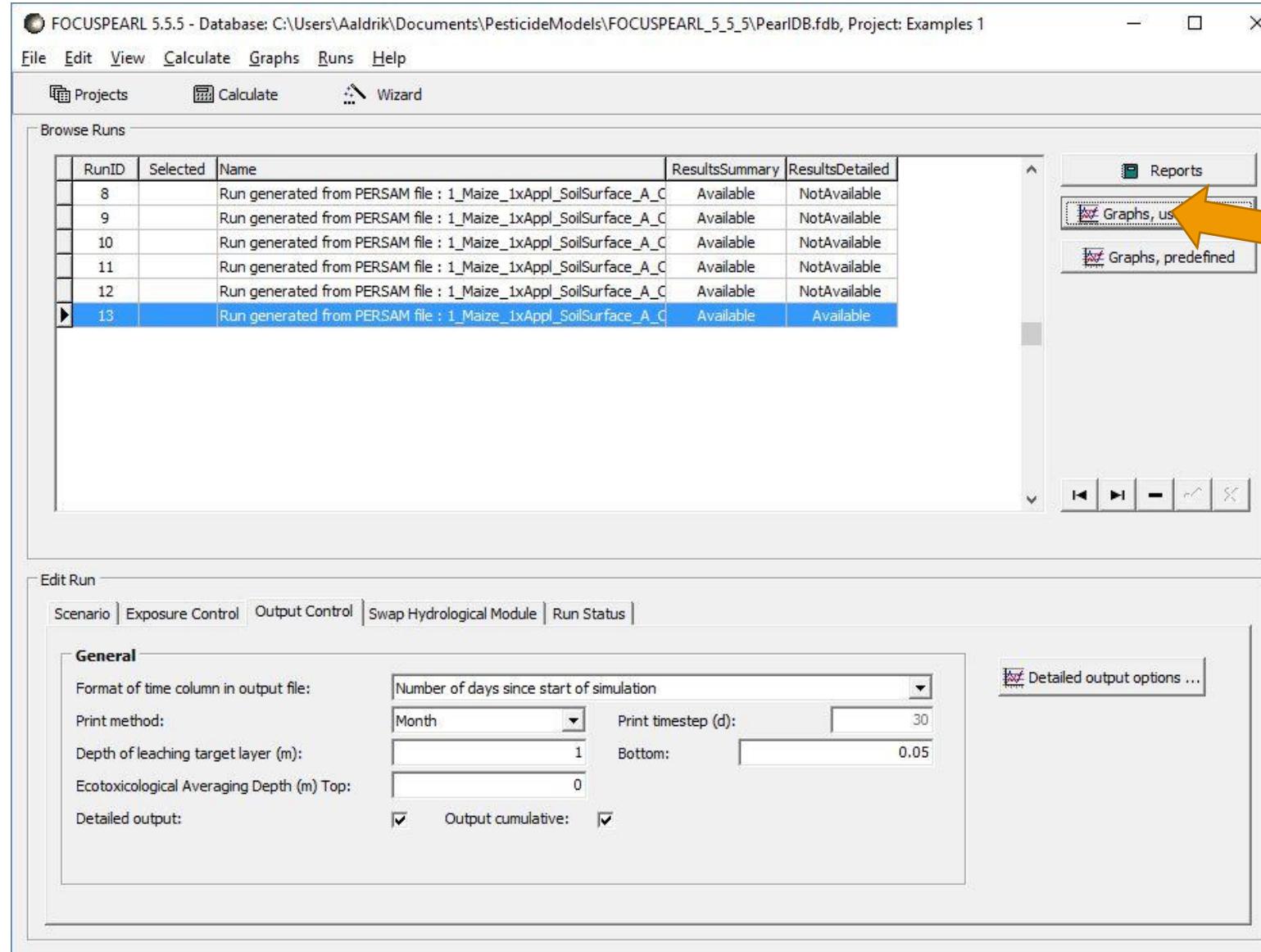
Ecotoxicological Averaging Depth (m) Top: 0

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
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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

Detailed output options ...

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

Ecotoxicological Averaging Depth (m) Top: 0

Detailed output: Output cumulative:

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
	Areic mass of substance applied to the soil		No	No	No
	Areic mass of substance in the equilibrium domain of the soil profile		No	Yes	No
	Areic mass of substance in the equilibrium domain of the FOCUS layer		No	Yes	No
	Areic numerical mass balance error		No	Yes	No
	Areic mass of substance formed		No	Yes	No
	Areic mass of substance in the non-equilibrium domain of the soil profile		No	Yes	No
	Areic mass of substance in the non-equilibrium domain of the FOCUS layer		No	Yes	No
Yes	Areic mass of substance in the equilibrium domain of the soil profile		No	Yes	No
	Areic mass of substance in the FOCUS layer		No	Yes	No
	Areic mass of substance transformed		No	Yes	No

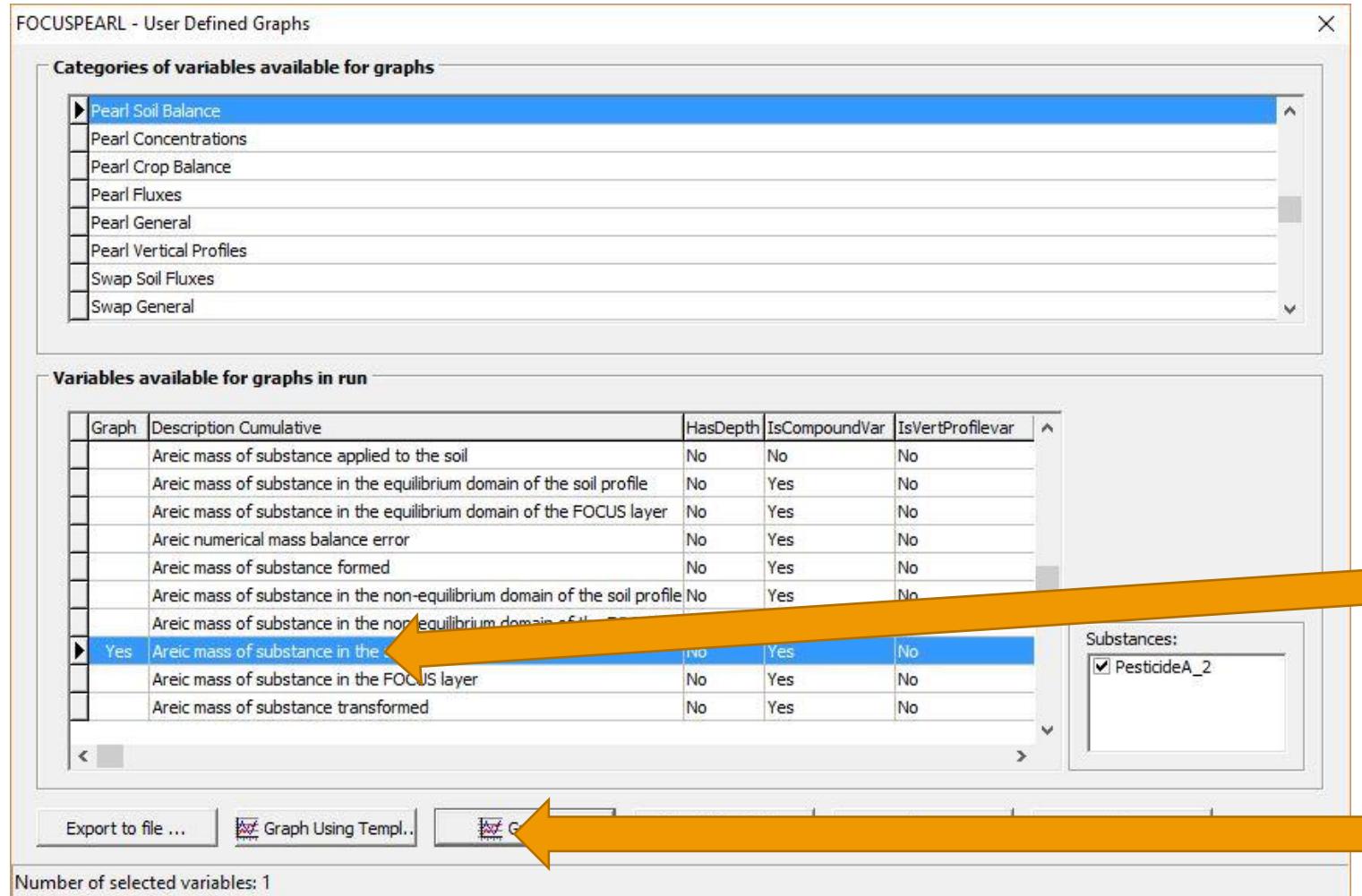
Substances:

- PesticideA_2

Export to file ...

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

