



## **4. DEMO AND EXERCISES**

**FROGS (French Refinement Of Groundwater Scenarios)  
UIPP Training**

**Paris, 16 November 2011**

**UIPP Environmental Methodology Working Group**



## 1. Introduction to FROGS GUI

- Create FROGS project
- Run and Evaluate FROGS

## 2. FROGS Mitigation Sheet

Password-protected download from webpage  
(<http://frogs.eclosion-share.net/>)  
(10GB due to stored hydrology)



### French Refinement Of Groundwater Scenarios

The FROGS groundwater scenarios and model interface have been developed as a higher-tier tool for the French pesticide registration procedure. These national scenarios are intended for the assessment of the risk of Plant Protection Products' active substances and their metabolites to leach to groundwater. They are currently available for use on winter wheat, winter barley, oilseed rape, maize fodder, maize grain, sugar beet, potato and sunflower. The scenarios were generated to reflect typical realistic conditions and practices under which arable crops are grown in France. They consist of the combination of a limited number of Agronomic Units (AU, homogeneous geographic entities which show common agricultural and physical conditions) associated to representative soil, weather, crop rotations and phenological information. The work was initiated by the INRA SSM ComTox precursor workgroup on French groundwater scenarios (Commission d'étude de la toxicité - Sous-groupe environnement - Atelier ESO), and continued by a dedicated UIPP workgroup who finalized the scenarios and produced a workable tool, including a database where all input parameters are stored in a transparent way and a user-friendly model interface to be used in combination with the groundwater model PEARL. FROGS can be freely downloaded from this website.

Documentation

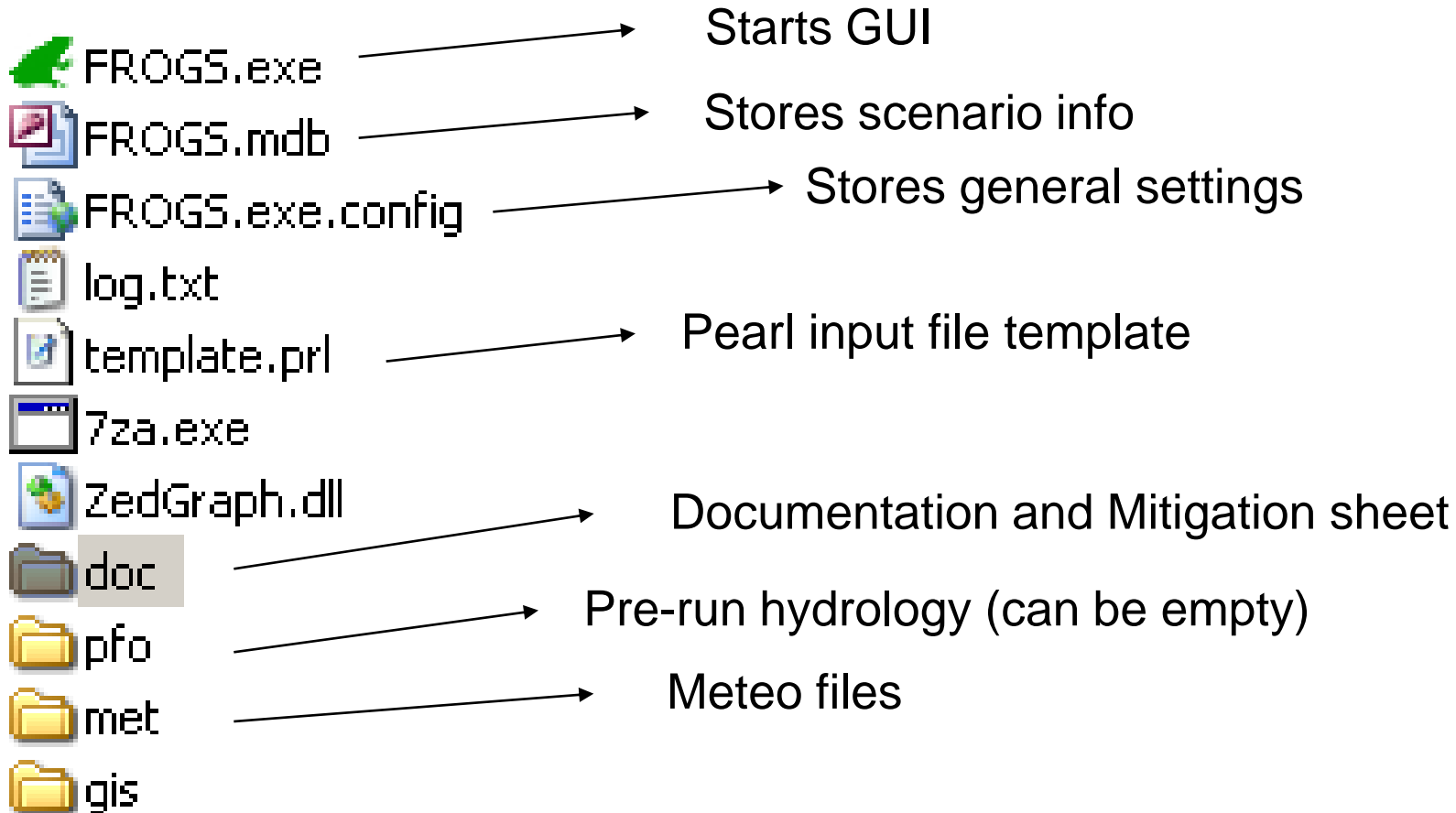
Training material

Download FROGS

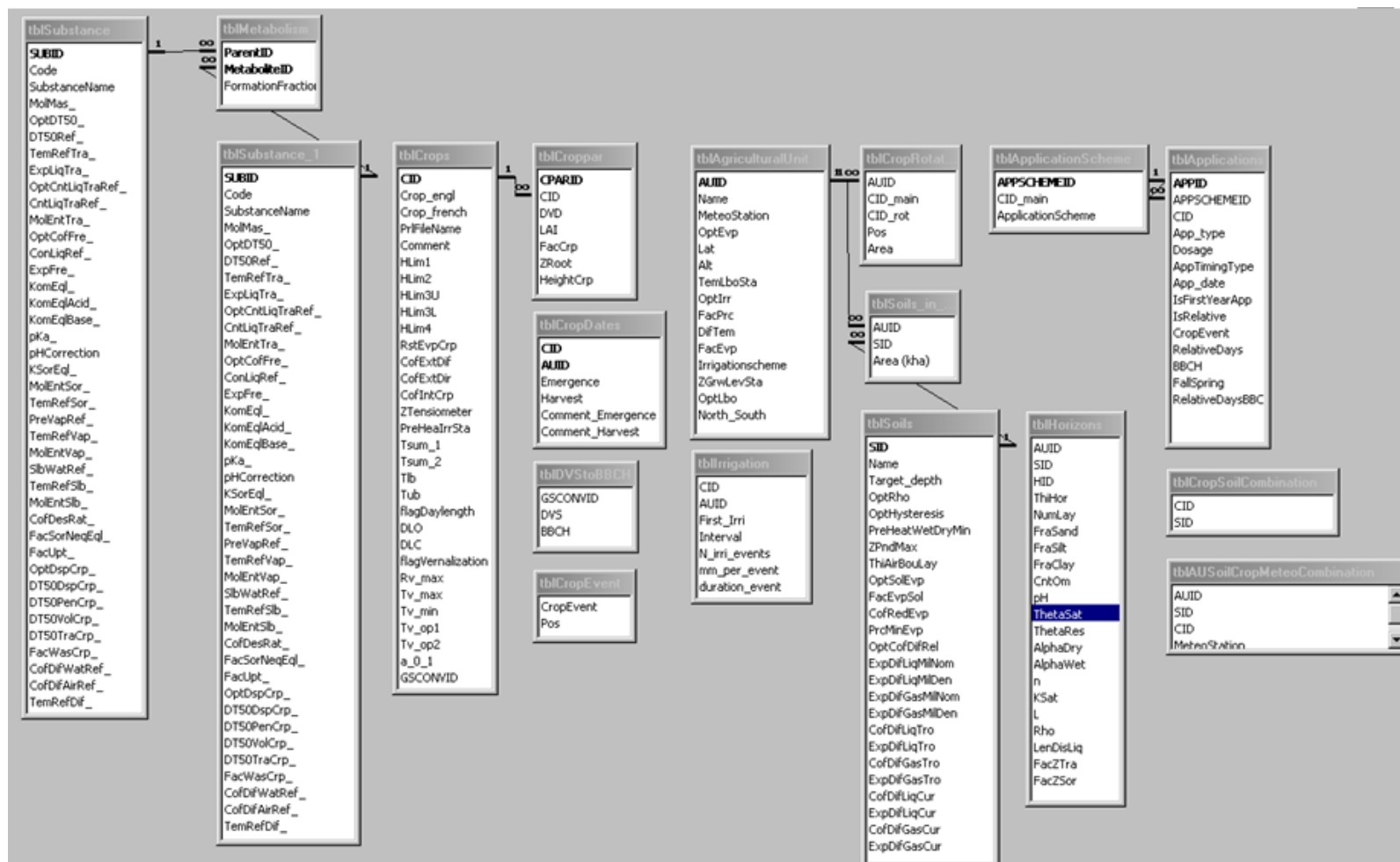
#### Training Material

- 1 Introduction
  - 2.1 Methodology Agronomic Units
  - 2.2 Methodology crops
  - 2.3 Methodology meteo and irrigation
  - 2.4 Methodology soil
  - 3 Implementation in French evaluation scheme
  - 4 Demo and Exercises
  - 5 Conclusions
- (version 29.10.2010)

[ Contact us ]



**! pearlmodel.exe/swap209e.exe have to be available on your computer !**  
**! No PEARL installation necessary !**



```

TextPad - [M:\Personal Data\Projects\FROGS\tool\download28_01_2011\FROGS\template.prl]
Datei Bearbeiten Suchen Ansicht Extras Makros Konfiguration Fenster Hilfe

*-----*
* INPUT FILE for PEARL
* Generated by FGWS on #CREATION DATE#
#RUN INFO#
*-----*

* Section 1: Control section
*-----*

FOCUS CallingProgram
3 ModelVersion
3 GUIVersion
3 DBVersion
6 InitYears
#TimStart# TimStart
#TimEnd# TimEnd
0.0 AmaSysEnd (kg.ha-1)
0.001 ThetaTol (m3.m-3)
Other OptDelTimPrn
1 DelTimPrn (d)
No RepeatHydrology
Automatic OptHyd
1E-7 DelTimSwaMin (d)
0.2 DelTimSwaMax (d)
Yes PrintCumulatives
1.0 GWLTol (m)
1000000 MaxItSwa
No OptHysteresis
0.2 PreHeaWetDryMin (cm)
Yes OptScreen

*-----*
* Section 2: Soil section
*-----*

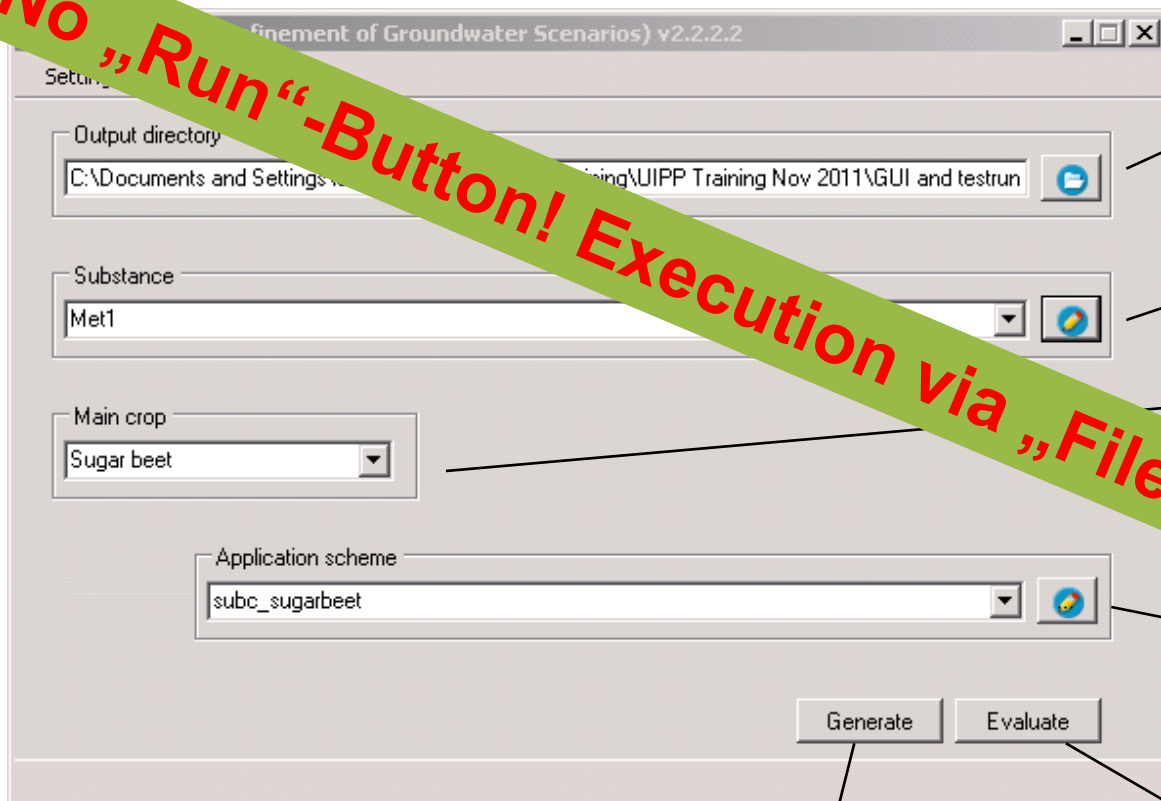
```



### Initial Settings (to be adjusted only once)



**No „Run“-Button! Execution via „File-Manager“ necessary**



Working directory for in – and output

Substance definition

Crop for which PEC-calculations are performed

Define Application Scheme

Generates Input files in working directory

Evaluates output files from working directory



Application settings

Pri-File template  
template.prl

Path to "met" folder  
met

Path to pearlmodel.exe  
C:\Program Files\Focuspearl\_3\_3\_3\bin\pearlmodel.exe

Path to database  
FROGS.mdb

Path to "pfo" folder  
pfo

Pre-run hydrology  
 Copy hydrology to output directory?

Save & Exit Exit



Check if runs are to be executed  
at different computer/location

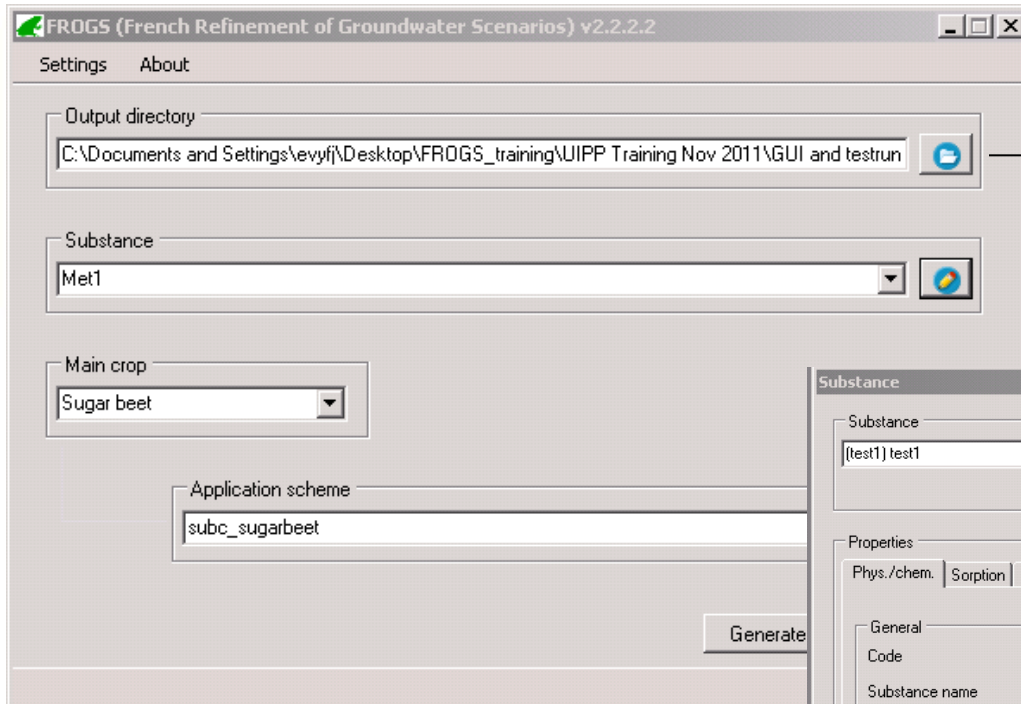
Location of pre-run hydrology files  
(has to be specified even if \*.pfo files  
are not used)



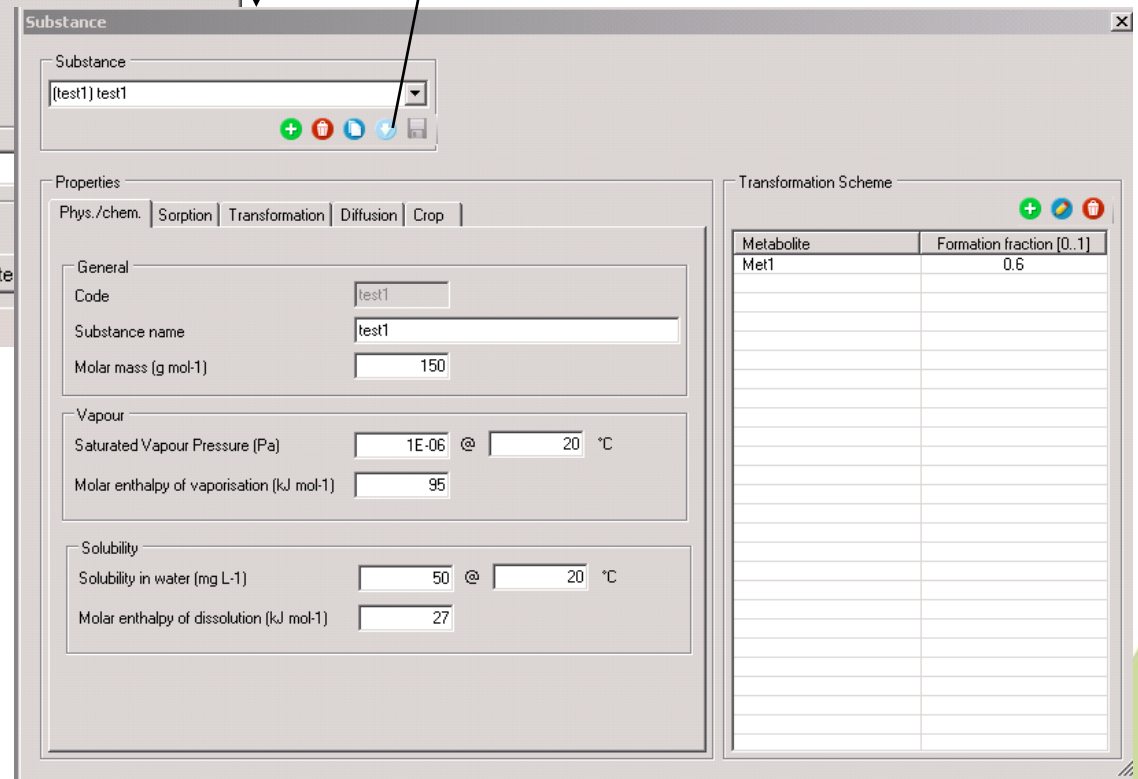
### Exercise 1:

- **Adjust Initial Settings**
- **Create working directory for 2 projects:**
  - **Substance SubC in Sugar Beet**
  - **Substance Test1 in Winter Wheat**





Option to import existing \*.prl files



Formation fractions are not imported → enter manually after import

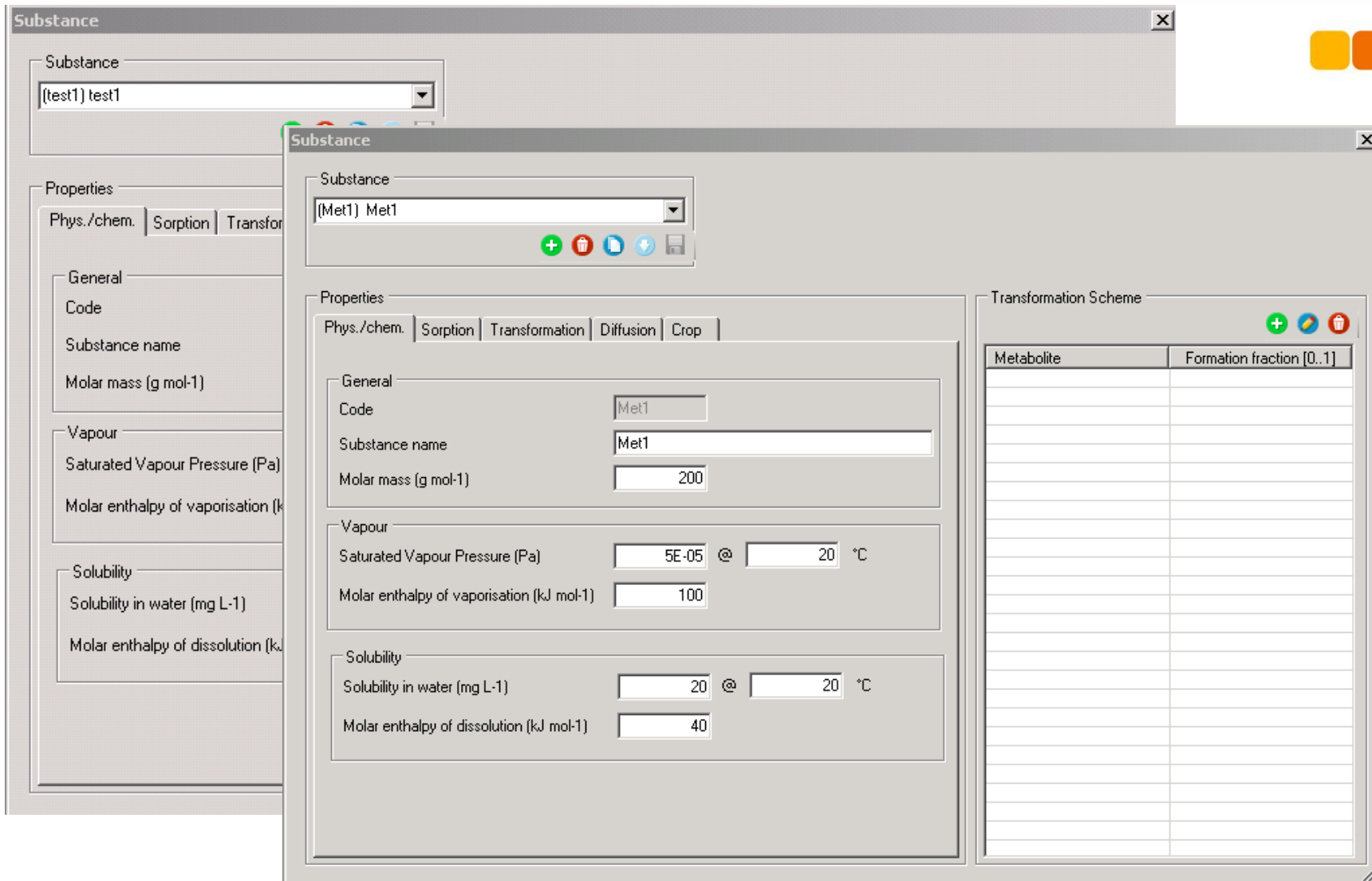


### Exercise 2:

- **Create your substance of choice manually**
- **Import substance test1.prl (in folder „Exercise“)**
  - **with metabolite; don't forget to adjust formation fraction**
  - **necessary for test runs**



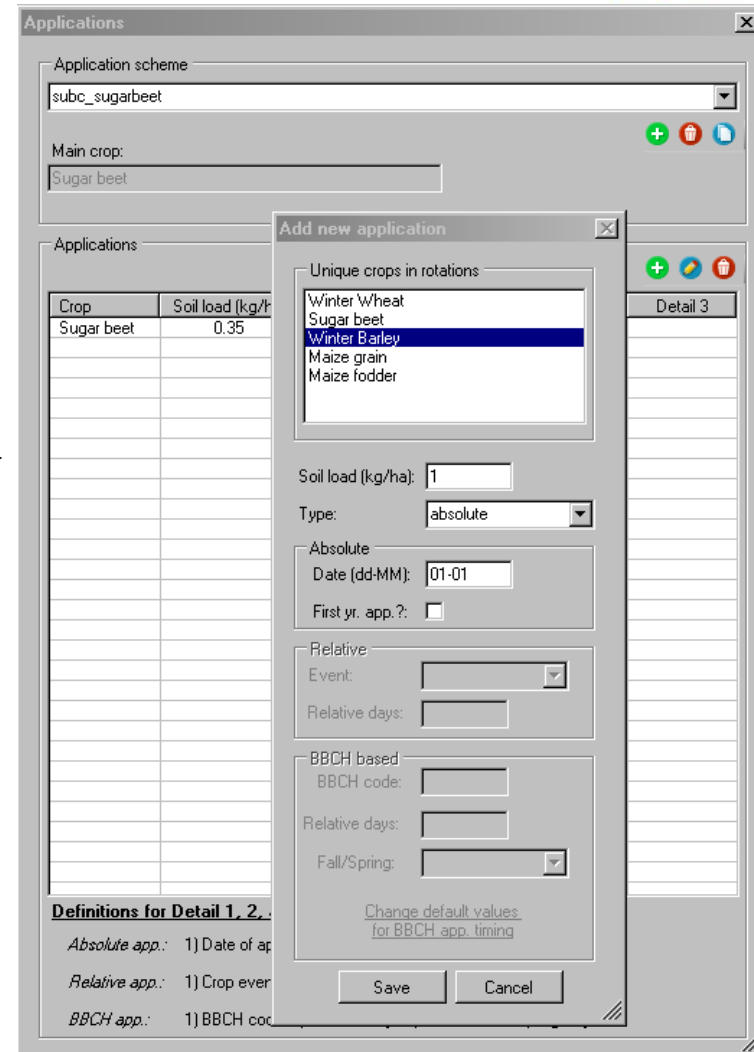
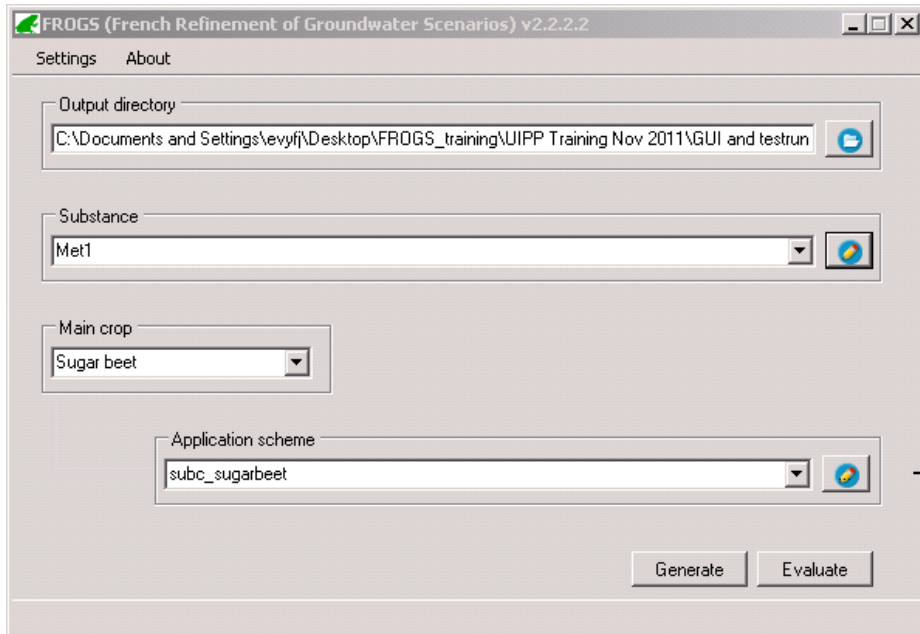
Parameter	SubC		Test1	
	Parent	Metabolite	Parent	Metabolite
Formation fraction	-	0.71	-	0.6
DT50 (d)	20	100	80	30
Kom (L/kg)	100	30	90	120
1/n	0.9	0.9	0.9	0.9
Solubility (mg/L)	50	90	50	20
Molar weight (g/mol)	200	150	150	200
Vapour pressure (Pa)	1E-10	1E-10	1E-6	5E-5
Mol. Enth. of Vapor. (kJ/mol)	95	95	95	95
Mol. Enth. of Diss. (kJ/mol)	27	27	27	27
Activation energy (kJ/mol)	65.4	65.4	65.4	65.4



The screenshot displays the 'Substance' dialog box in a software application. The dialog is divided into several sections:

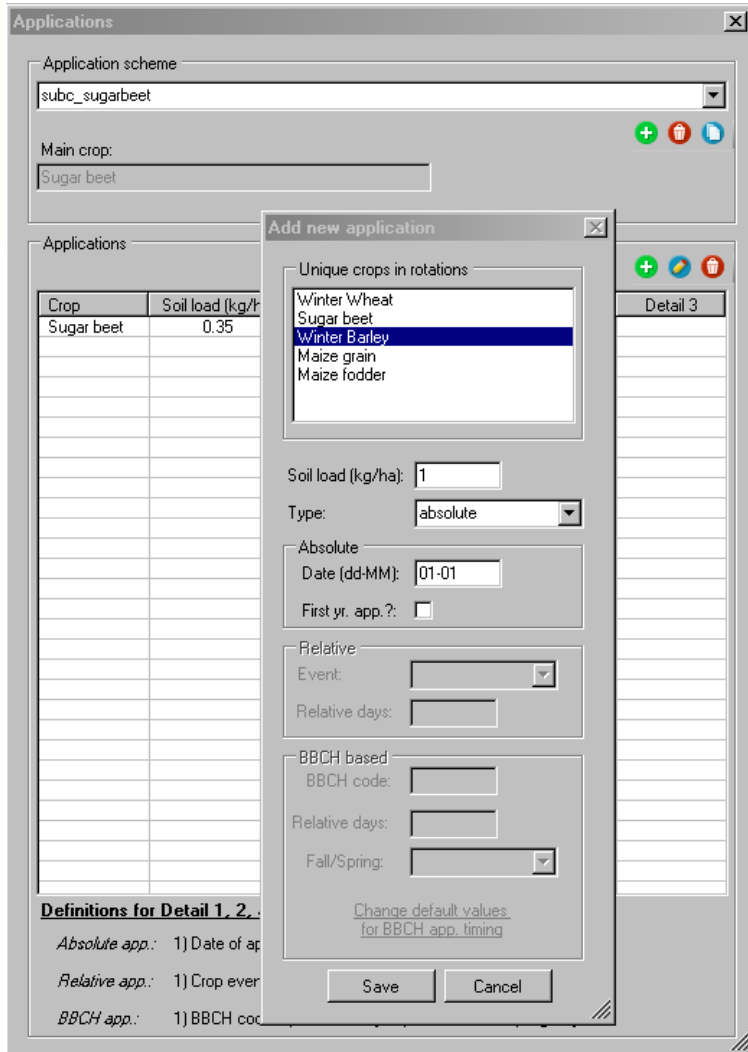
- Substance:** A dropdown menu showing '(test1) test1'.
- Properties:** A tabbed interface with 'Phys./chem.' selected. It contains:
  - General:** Code (Met1), Substance name (Met1), Molar mass (g mol<sup>-1</sup>) (200).
  - Vapour:** Saturated Vapour Pressure (Pa) (5E-05) @ 20 °C, Molar enthalpy of vaporisation (kJ mol<sup>-1</sup>) (100).
  - Solubility:** Solubility in water (mg L<sup>-1</sup>) (20) @ 20 °C, Molar enthalpy of dissolution (kJ mol<sup>-1</sup>) (40).
- Transformation Scheme:** A table with two columns: 'Metabolite' and 'Formation fraction [0..1]'. The table is currently empty.





Each Application scheme consists of 1 – X applications

First year application: for bi-annual crops → defines in which year (1st or 2nd) application is done  
 (Before December = check  
 From January on = uncheck)



Crop	Soil load (kg/ha)
Sugar beet	0.35

**Definitions for Detail 1, 2, ...**

- Absolute app.: 1) Date of ap
- Relative app.: 1) Crop ever
- BBCH app.: 1) BBCH coc

- Application should (in theory) be always made to all crops in the GAP-list
- For winter cereals: two runs (ww and barley) always applied to both crops
- For maize: two runs (fodder and grain maize) always applied to both crops





### Exercise 3:

- **Update the existing scheme „subC\_Sugarbeet“: Add two more applications to sugar beet (0.35 kg/ha, first application at day of emergence, 5 days interval)**
  - **Create Scheme for substance Test1 on winter wheat:**
    - 80 g/ha, 5 days before emergence (applied on both winter wheat and winter barley)
- ➔ Both needed for test runs





### Exercise 3 (continued):

If you still have time left...

Enter following application scheme for winter oilseed rape as main crop and without considering crop interception:

- **winter oilseed rape**
  - 2 applications with 7 days interval starting 5 days before emergence (each 0.2 kg/ha)
- **winter wheat**
  - 1 application always 1<sup>st</sup> December (0.15 kg/ha)
- **winter barley**
  - 3 applications at BBCH 39-69 with 10 days interval (each 0.1 kg/ha)

### „subC\_Sugarbeet“



**Applications** ✕

---

Application scheme

Main crop:

---

Applications

Crop	Soil load (kg/ha)	Type	Detail 1	Detail 2	Detail 3
Sugar beet	0.35	relative	Emergence	0 days	
Sugar beet	0.35	relative	Emergence	5 days	
Sugar beet	0.35	relative	Emergence	10 days	

„test1\_wc“



**Applications** ✕

---

Application scheme

test1\_wc ▼

+ ✖ 📄

Main crop:

Winter Wheat

---

Applications 
+ 🖌️ ✖

Crop	Soil load (kg/ha)	Type	Detail 1	Detail 2	Detail 3
Winter Wheat	0.08	relative	Emergence	-5 days	
Winter Barley	0.08	relative	Emergence	-5 days	

### „exercise\_data\_entry“



**Applications** ✕

---

Application scheme

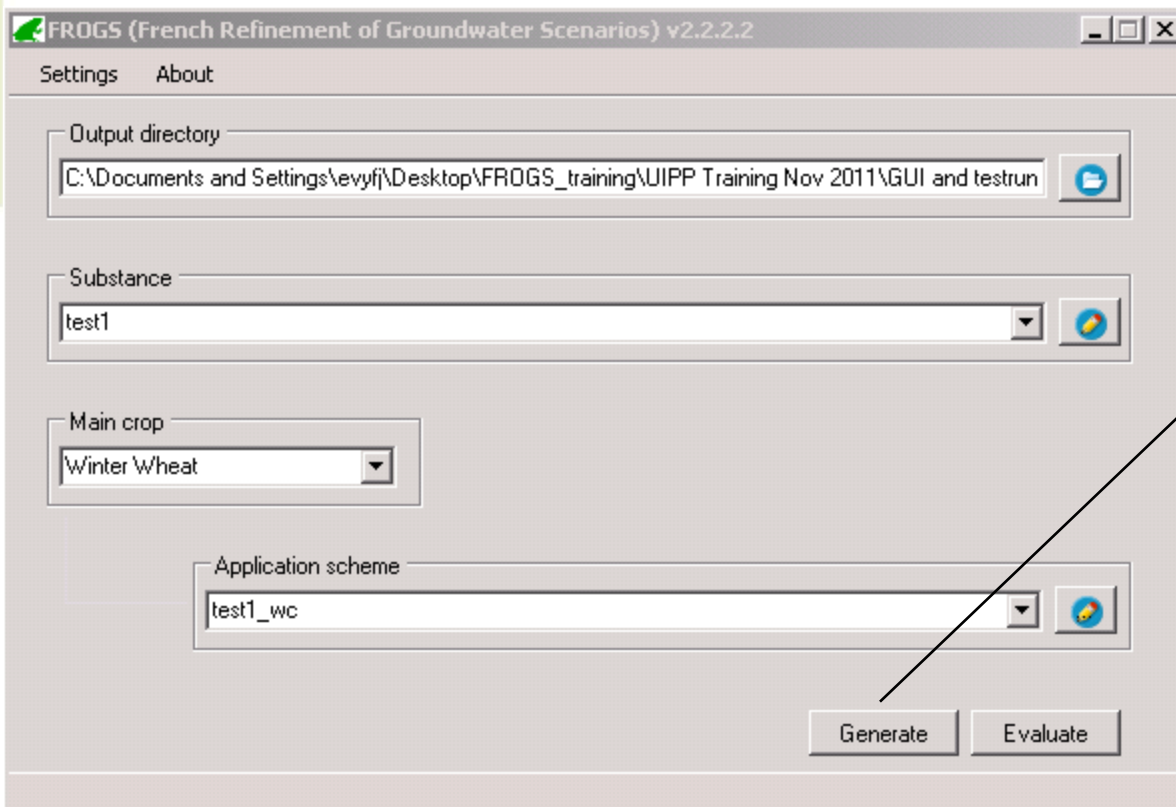
+
✖
📄

Main crop:

---

Applications 
+
✎
✖

Crop	Soil load (kg/ha)	Type	Detail 1	Detail 2	Detail 3
Oil seed rape	0,2	relative	Emergence	-5 days	
Oil seed rape	0,2	relative	Emergence	2 days	
Winter wheat	0,15	absolute	01-12	1st yr	
Winter Barley	0,1	BBCH	39	0	.
Winter Barley	0,1	BBCH	39	10	.
Winter Barley	0,1	BBCH	39	20	.



After defining all details click „Generate“ to generate all input.

→ Allows modification/distribution of runs before execution

Then open output directory with any „File manager“  
→ Start FROGS by clicking „run.bat“

Name	Size	Type
1.prl	31 KB	PRL File
1.SWE	0 KB	SWE File
2.prl	32 KB	PRL File
2.SWE	0 KB	SWE File
3.prl	32 KB	PRL File
3.SWE	0 KB	SWE File



PEARL input files, \*.swe tells PEARL that SWAP-output is available

53050.met	580 KB	MET File
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Meteo files

AUID 31 SID 12 CID 2.7z	3,166 KB	WinRAR-Archiv
AUID 31 SID 13 CID 2.7z	3,581 KB	WinRAR-Archiv
AUID 31 SID 19 CID 2.7z	3,299 KB	WinRAR-Archiv
catalogue.txt	4 KB	Text Document
run.bat	33 KB	MS-DOS Batch File

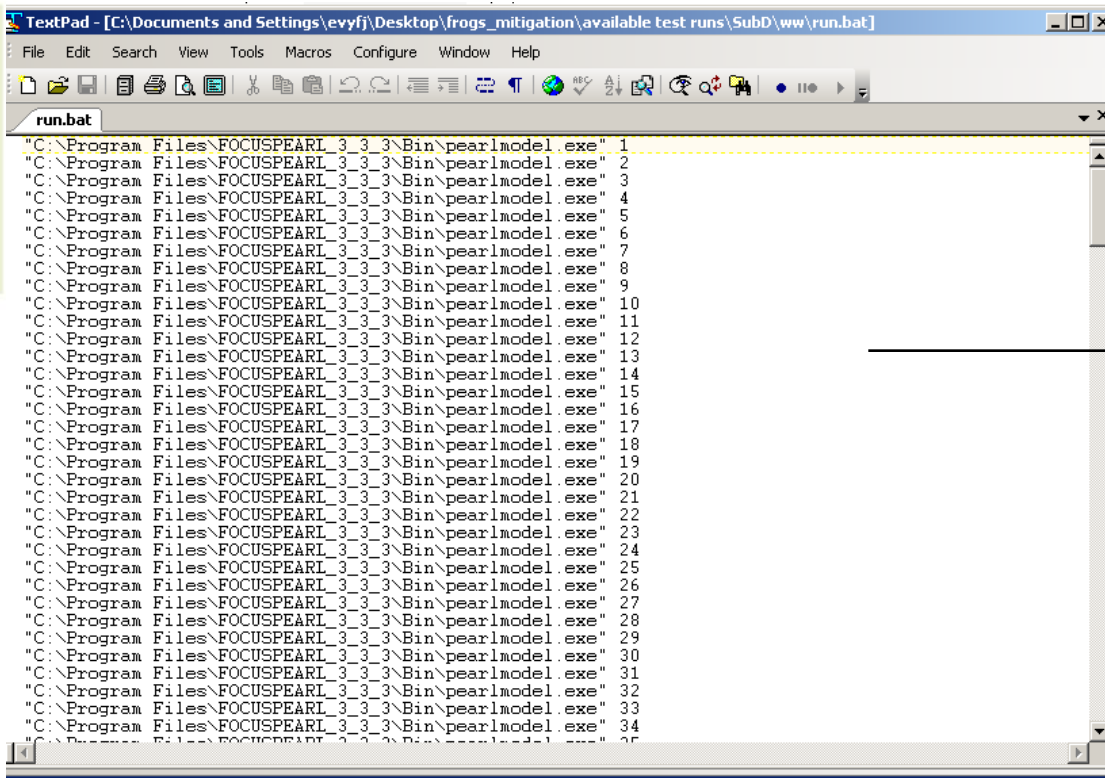
Zipped \*.pfo files

Summary of all runs

Batch file to run FROGS

7.SWE	0 KB	SWE File
7za.exe	524 KB	Application
7z.exe	22 KB	Application

Program to unzip \*.pfo files



```

run.bat
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 1
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 2
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 3
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 4
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 5
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 6
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 7
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 8
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 9
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 10
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 11
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 12
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 13
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 14
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 15
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 16
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 17
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 18
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 19
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 20
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 21
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 22
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 23
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 24
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 25
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 26
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 27
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 28
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 29
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 30
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 31
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 32
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 33
"C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 34

```

No \*.pfo files available → SWAP will be executed

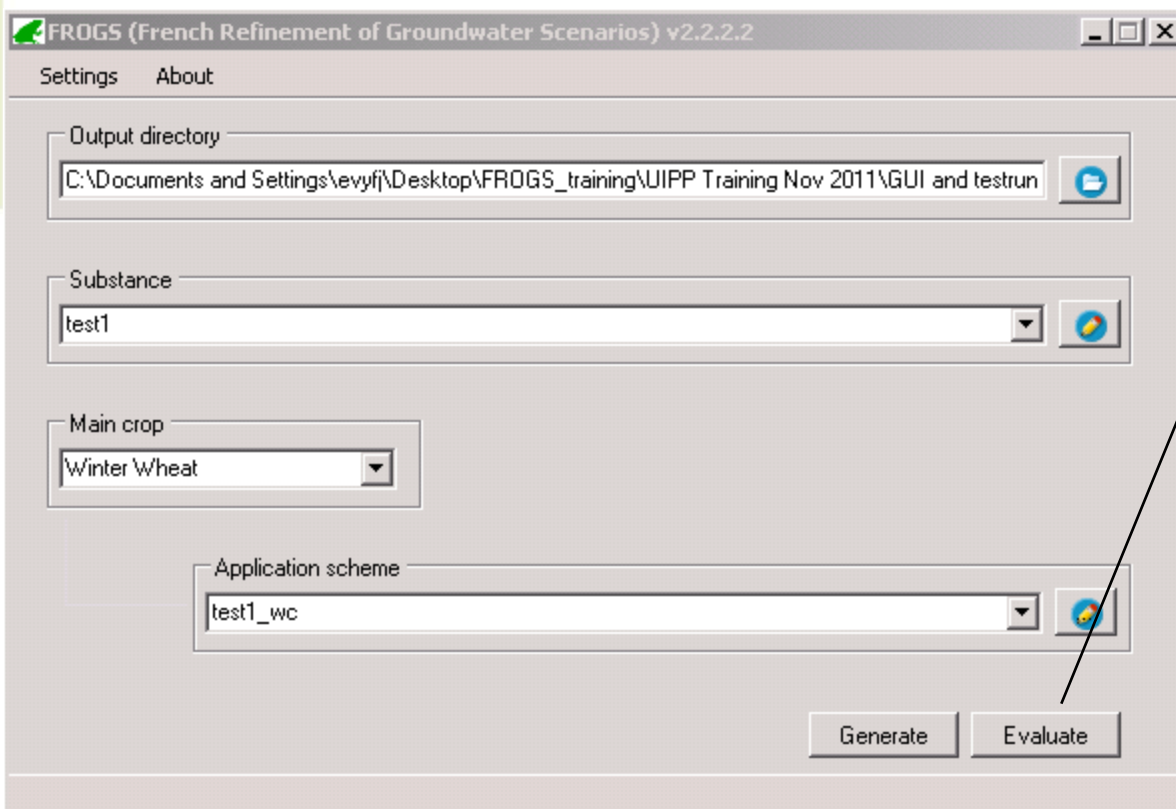
```

1 7za e "AUID 1 SID 1 CID 2.7z"
2 RENAME "AUID 1 SID 1 CID 2.pfo" 1.pfo
3 "C:\Program Files\FOCUSPEARL_3_3_3\Bin\pearlmodel.exe" 1
4 DEL /Q 1.pfo

```

\*.pfo files available → unzipping and renaming of \*.pfo files, SWAP is skipped → saves run-time

**Double click „run.bat“ to start FROGS runs**



After running FROGS click „Evaluate“ to create output files (necessary are only \*.sum files and catalogue.txt)

Output files:  
“**FROGS summary.txt**“  
“FROGS Cumulative Areal distribution - Sub-X.txt” and “-.png”



\*\*\*\* Main crop  
Sugar beet (SBEET)

\*\*\*\* Compounds

SubC	MET-C		
MolMas_*	200	150	(g.mol-1) Molar mass [10 10000]
OptDT50_*	Input	Input	Option for DT50: Input or Calculate
DT50Ref_*	20	100	(d) Half-life time [1 1e6]
TemRefTra_*	20	20	(C) Temperature at which DT50 is measured [5 30]
ExpLiqTra_*	0.7	0.7	(-) Exponent for the effect of liquid [0 5]
OptCntLiqTraRef_*	opt.	opt.	OptimumConditions (opt.) or NonOptimumConditions (non-opt.)
CntLiqTraRef_*	1	1	(kg.kg-1) Liq. content at which DT50 is measured [0 1]
MolEntTra_*	65.4	65.4	(kJ.mol-1) Molar activation energy [0 200]
OptCofFre_*	pH-independent	pH-independent	pH-dependent, pH-independent, CofFre
ConLiqRef_*	1	1	(mg.L-1) Reference conc. in liquid phase [0.1 -]
ExpFre_*	0.9	0.9	(-) Freundlich sorption exponent [0.1 1.3]
KomEqL_*	100	30	(L.kg-1) Coef. eql. sorption on org. matter [0 1e9]
KomEqLAcid_*	374.7	374.7	(L.kg-1) Coef. for eql. sorption on om - acid [0 1e9]
KomEqLBase_*	7.46	7.46	(L.kg-1) Coef. for eql. sorption on om - base [0 1e9]
pKa_*	4.6	4.6	(-) Coef. for influence of pH on sorption [0 14]
pHCorrection	0	0	(-) pH correction [-2 1]
KSorEqL_*	1	1	(L.kg-1) Coef. for equilibrium sorption [0 1e9]
MolEntSor_*	0	0	(kJ.mol-1)
TemRefSor_*	20	20	(C)
PreVapRef_*	1E-10	1E-10	(Pa) Saturated vapour pressure [0 2e5]
TemRefVap_*	20	20	(C) .. measured at [0 40]
MolEntVap_*	95	95	(kJ.mol-1) Molar enthalpy of vaporisation [-200 200]
SibWatRef_*	50	90	(mg.L-1) Solubility in water [1e-9 1e6]
TemRefSib_*	20	20	(C) .. measured at [0 40]
MolEntSib_*	27	27	(kJ.mol-1) Molar enthalpy of dissolution [-200 200]
CofDesRat_*	0	0	(d-1) Desorption rate coefficient [0 0.5]
FacSorNeqEql_*	0	0	(-) CofFreNeq/CofFreEql [0 -]
FacUpt_*	0.5	0.5	(-) Coefficient for uptake by plant [0 10]
OptDspCrp_*	Lumped	Lumped	Lumped or Specified
DT50DspCrp_*	1000000	1000000	(d) Half-life at crop surface [1 1e6]
DT50PenCrp_*	-	-	(d) Half-life due to penetration [1 1e6]
DT50VolCrp_*	-	-	(d) Half-life due to volatilization [1 1e6]
DT50TraCrp_*	-	-	(d) Half-life due to transformation [1 1e6]
FacWasCrp_*	0.0001	0.0001	(m-1) Wash-off factor [1e-6 0.1]
CofDifWatRef_*	4.3E-05	4.3E-05	(m2.d-1) Reference diff. coeff. in water [10e-5 3e-4]
CofDifAirRef_*	0.43	0.43	(m2.d-1) Reference diff. coeff. in air [0.1 3]
TemRefDif_*	20	20	(C) Diff. coeff measured at temperature [10 30]

-- Transformation scheme  
0.71 SubC -> MET-C

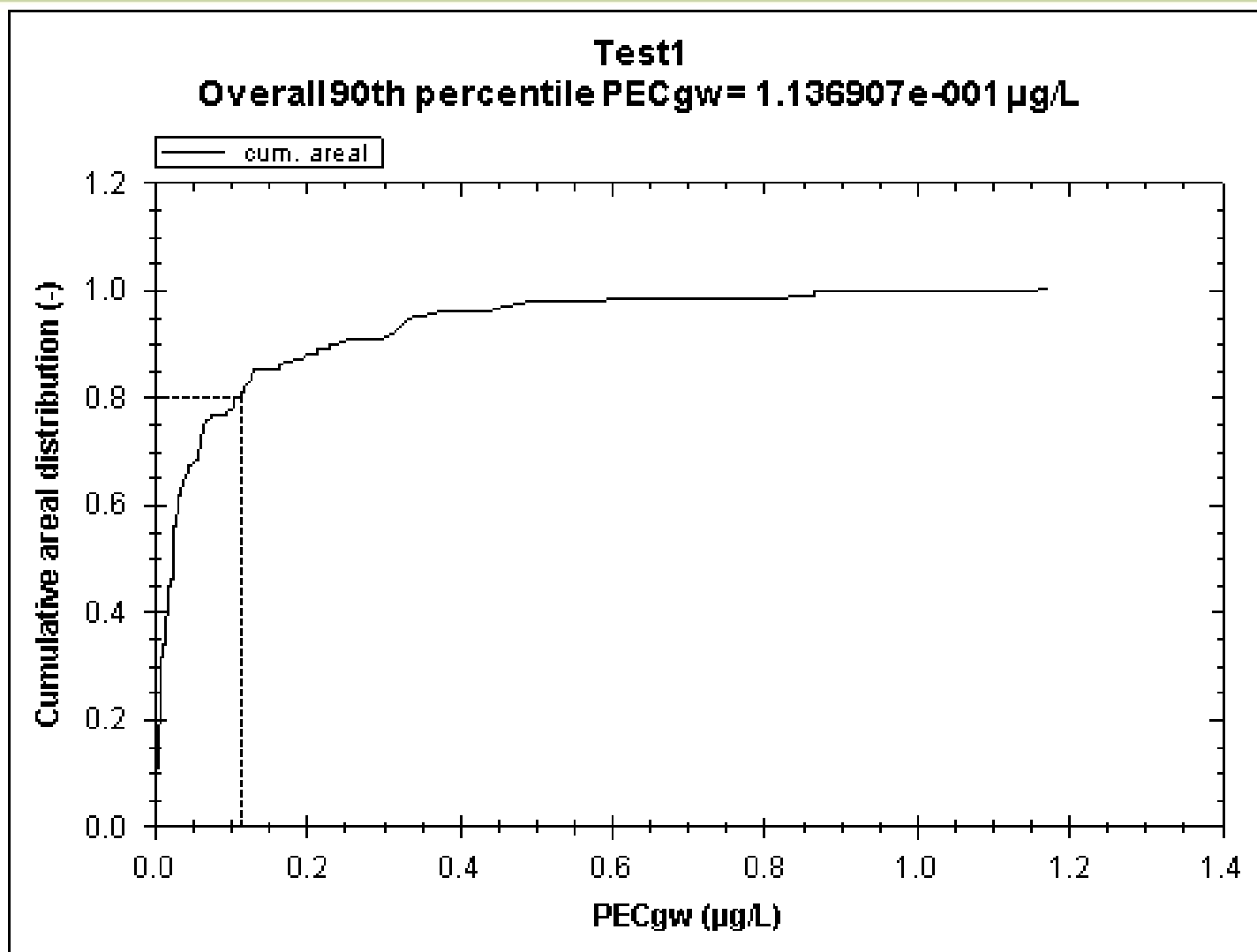
\*\*\*\* Application scheme "subc\_sugarbeet"

Crop	Soil load	Type	
SBEET	0.35	relative	Emergence 0 days

\*\*\*\* Results

RUNID	AUID	AU	SID	Soil	Area (kha)	Rotation	SUBID	Substance	80th percentile Year	Comment
1	4	Bordure Nord - Picardie	-	Normandie	1	Luvisol 3 >80 cm	6	SBEET-WWHEAT-WWHEAT	2	SubC 4.33717687843847E-10 1999
1	4	Bordure Nord - Picardie	-	Normandie	1	Luvisol 3 >80 cm	6	SBEET-WWHEAT-WWHEAT	3	MET-C 2.65108981426512 2011
2	5	Alsace - Sundgau	1	Luvisol 3 >80 cm	6	SBEET-MAIZEG-MAIZEG	2	SubC 8.192200908632E-12 2002		
2	5	Alsace - Sundgau	1	Luvisol 3 >80 cm	6	SBEET-MAIZEG-MAIZEG	3	MET-C 2.07586020048767 2005		
3	6	Plaine normande - Bessin	1	Luvisol 3 >80 cm	61	SBEET-WWHEAT-MAIZEF	2	SubC 3.24754393247544E-17 2020		

## FROGS Cumulative Areal distribution – Test1.png



80<sup>th</sup> spatial percentile of FROGS scenarios = 0.113 µg/L → mitigation necessary



### Exercise 4:

- **Create Runs for:**
  - **SubC on Sugar Beet (App. Scheme: SubC\_sugarbeet)**
  - **Test1 on Winter Wheat (App. Scheme: Test1\_wc)**
- **Execute only the first two PEARL runs (for time reasons)**
  - **Open/Edit „run.bat“ (do not double click) and delete all necessary entries**
  - **Or close „DOS“-window after 2nd run**
- **Evaluate results / compare PECs**

SubC (from file „FROGS Summary.txt“)



RunID	AUID	SID	Area	Rotation	SubID	Substance	PECgw	Year
1	4	1	571	SB-WW-WW	2	SubC	4E-8	2038
1	4	1	571	SB-WW-WW	3	MetC	9.44	2035
2	5	1	6	SB-MG-MG	2	SubC	1E-9	1990
2	5	1	6	SB-MG-MG	3	MetC	7.47	1993

Test1 (from file „FROGS Summary.txt“)

RunID	AUID	SID	Area	Rotation	SubID	Substance	PECgw	Year
1	4	1	7	WW-SF	5	Test1	0.0037	2001
1	4	1	7	WW-SF	6	Met1	0.001	2017
2	5	1	35	WW-MF-BA	5	Test1	0.0003	2005
2	5	1	35	WW-MF-BA	6	Met1	7.97E-5	2023



# Mitigation



Different mitigation options are possible (most related to soil properties), but not limited to:

exclusion of scenarios

- by location (AUs)
- with soils of high sand content
- with soils of low OC content
- with soils of low available water capacity (function of texture and profile depth → excluding shallow soils and high sand contents)

**! No additional runs have to be calculated, but existing results have to be filtered !**

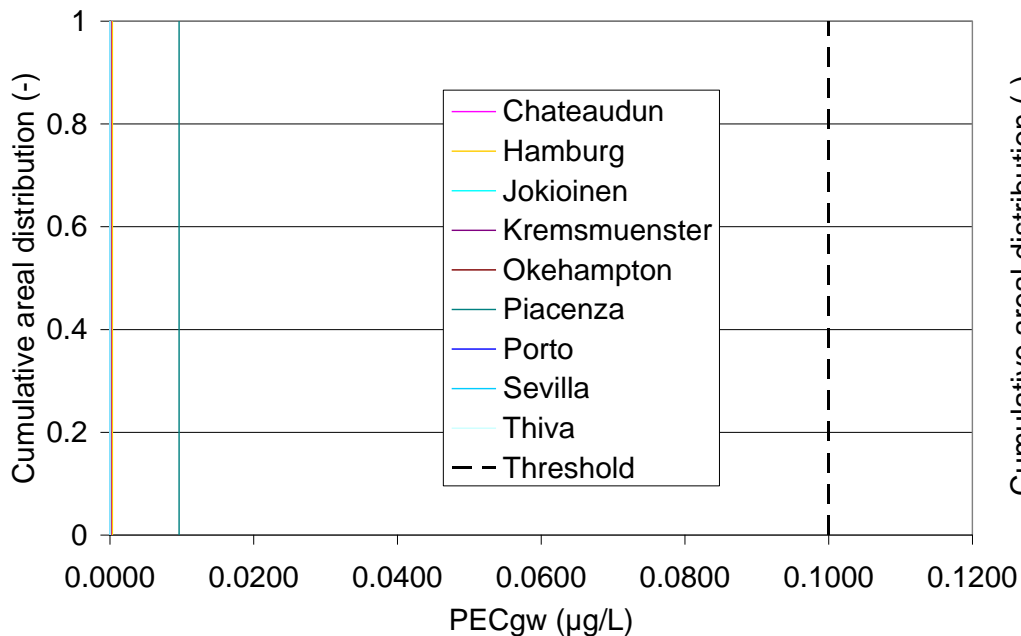
→ Use Excel-Sheet „FROGS template mitigation.xls“ to check and apply mitigation options



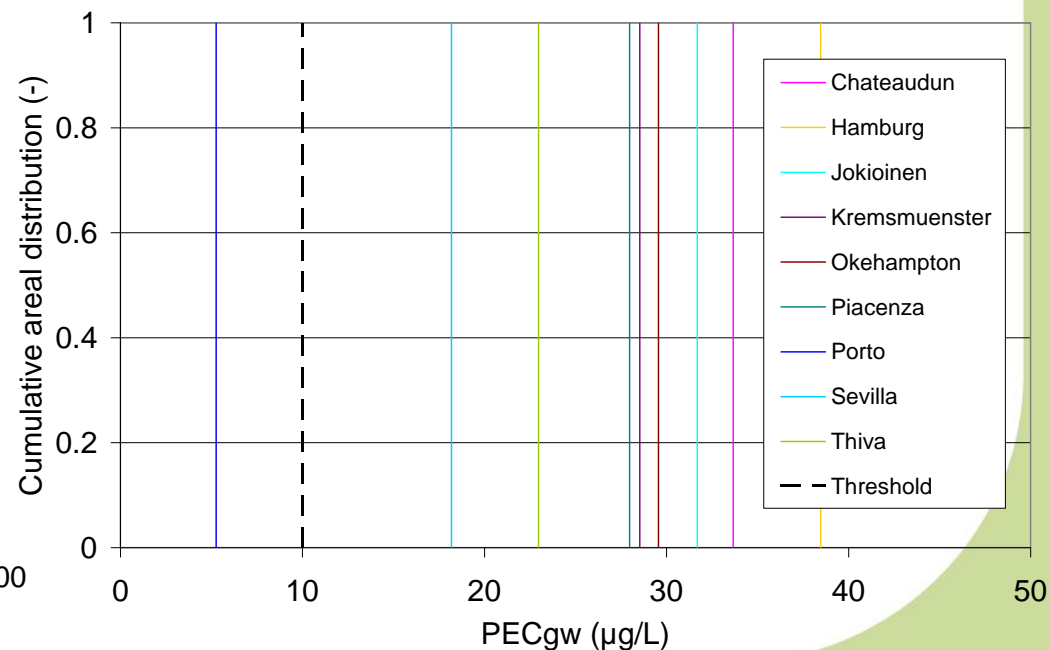
SubC in sugar beet

➔ (non-relevant) Metabolite exceeds threshold of 10 µg/L

Parent



Non-relevant Metabolite

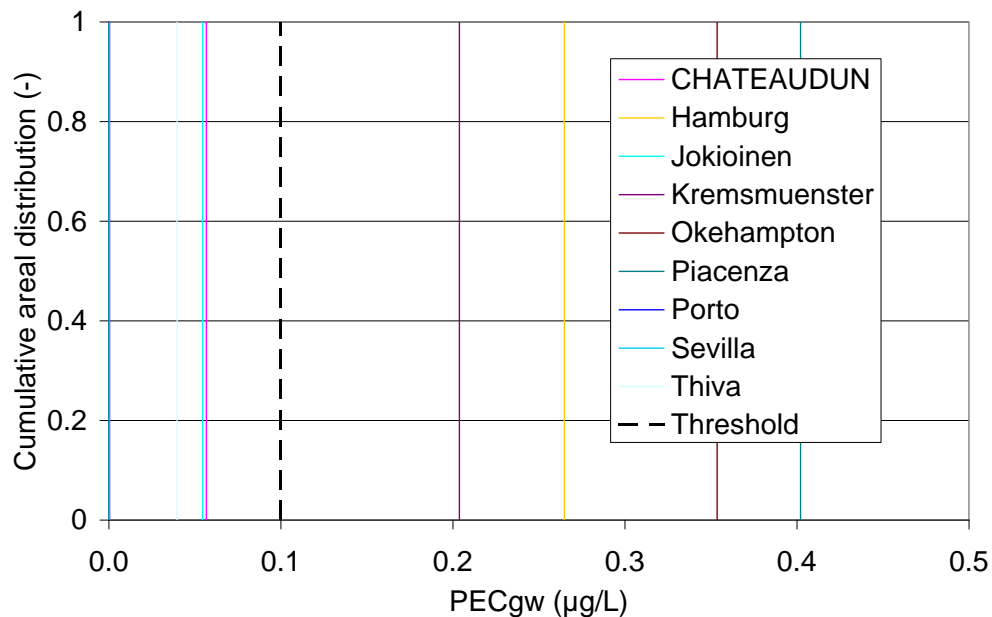




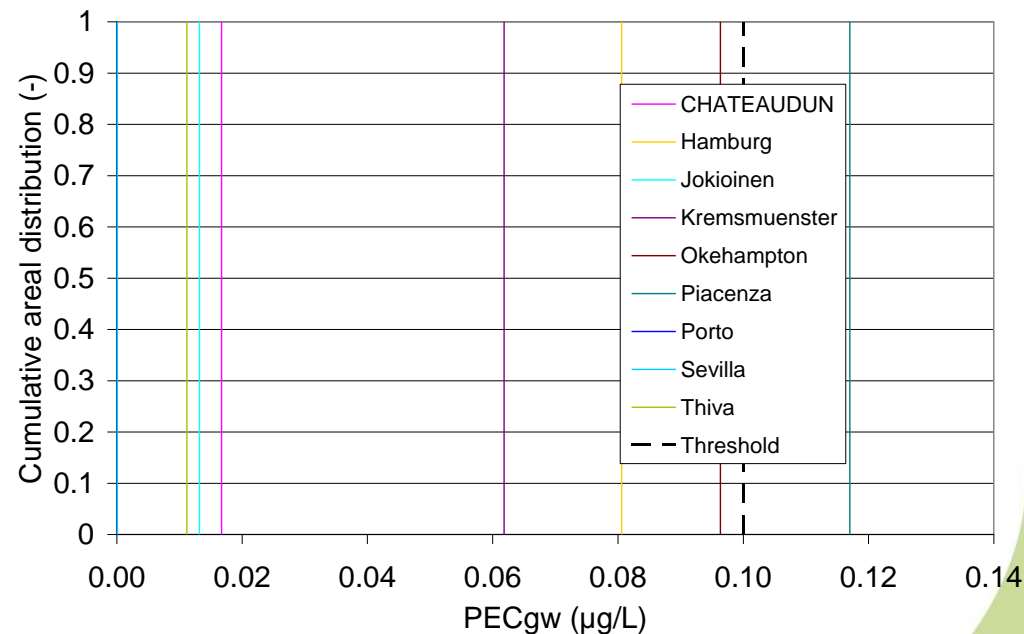
Test1 applied to winter wheat

➔ Parent and metabolite exceed threshold of 0.1 µg/L

### Parent

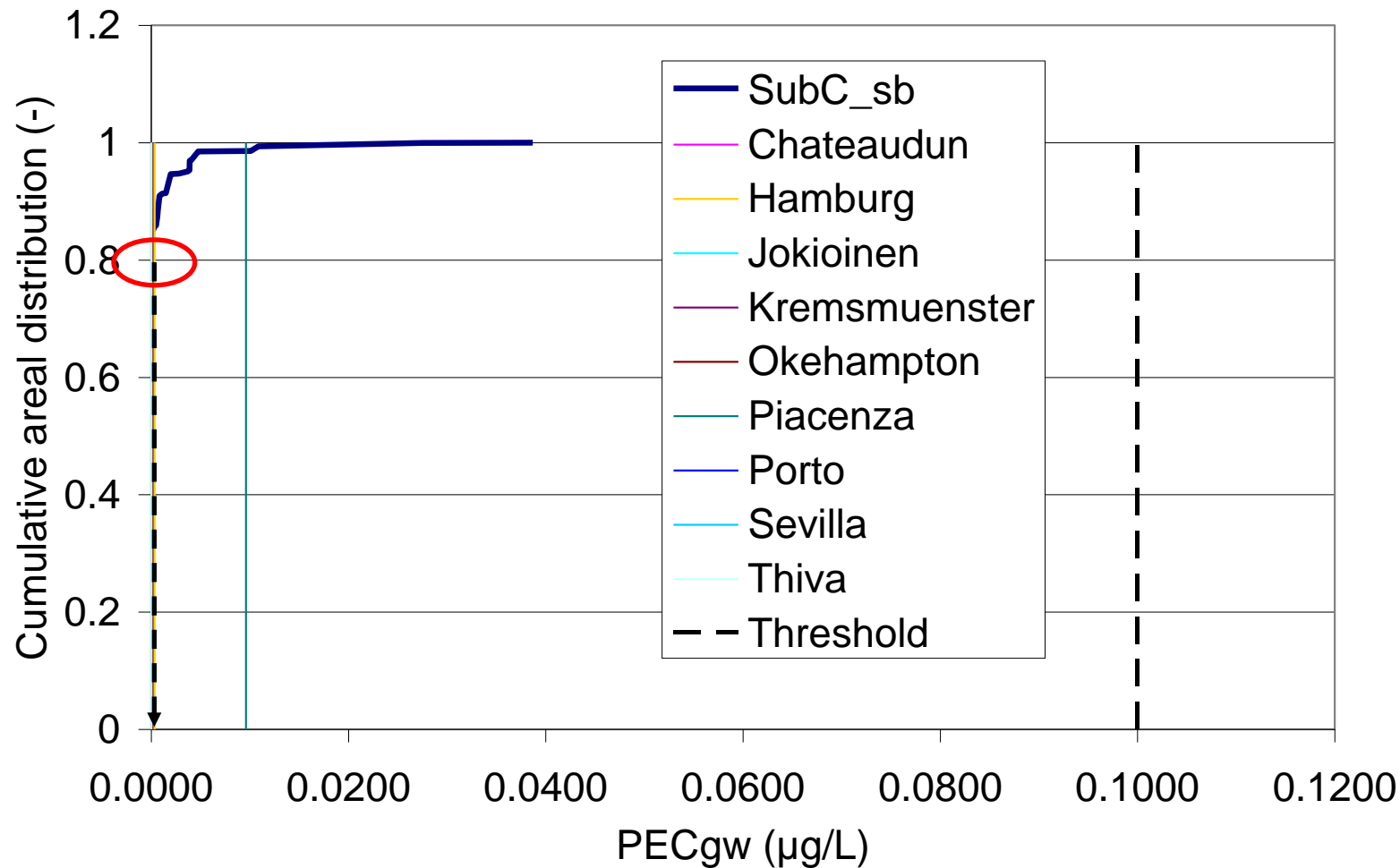


### (relevant) Metabolite



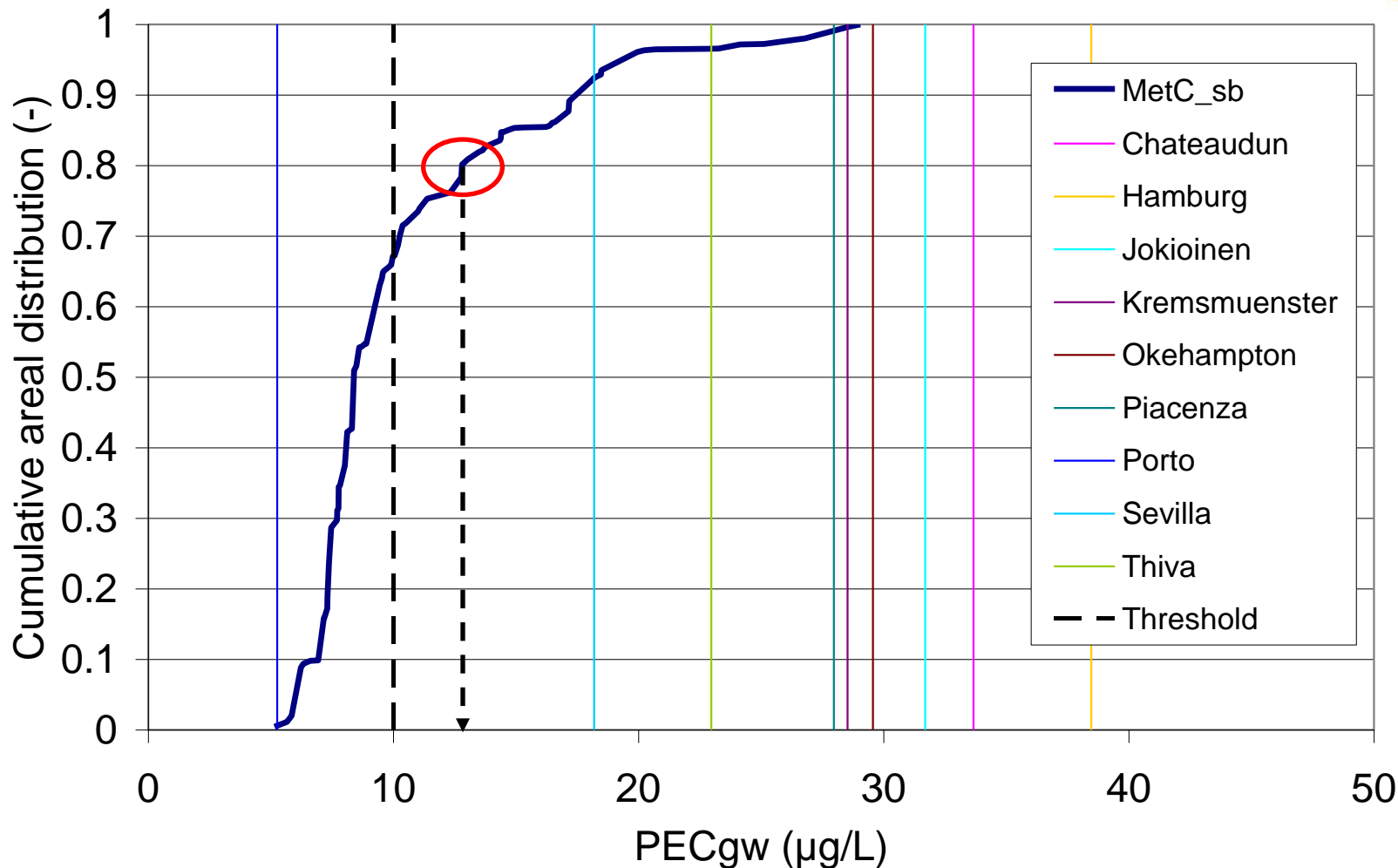


### Parent SubC



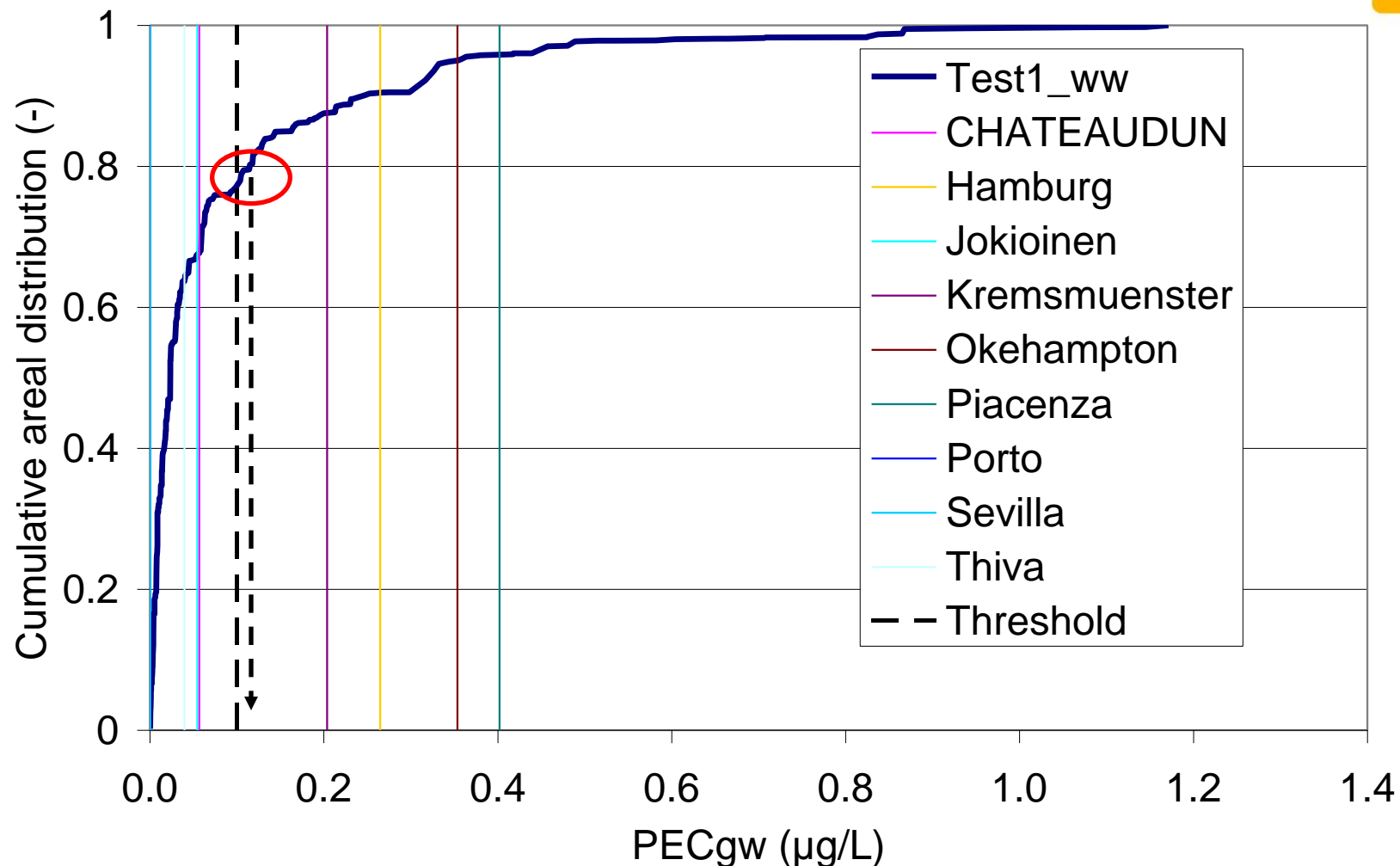
80<sup>th</sup> spatial percentile of FROGS scenarios < 0.1 µg/L

### Metabolite MetC

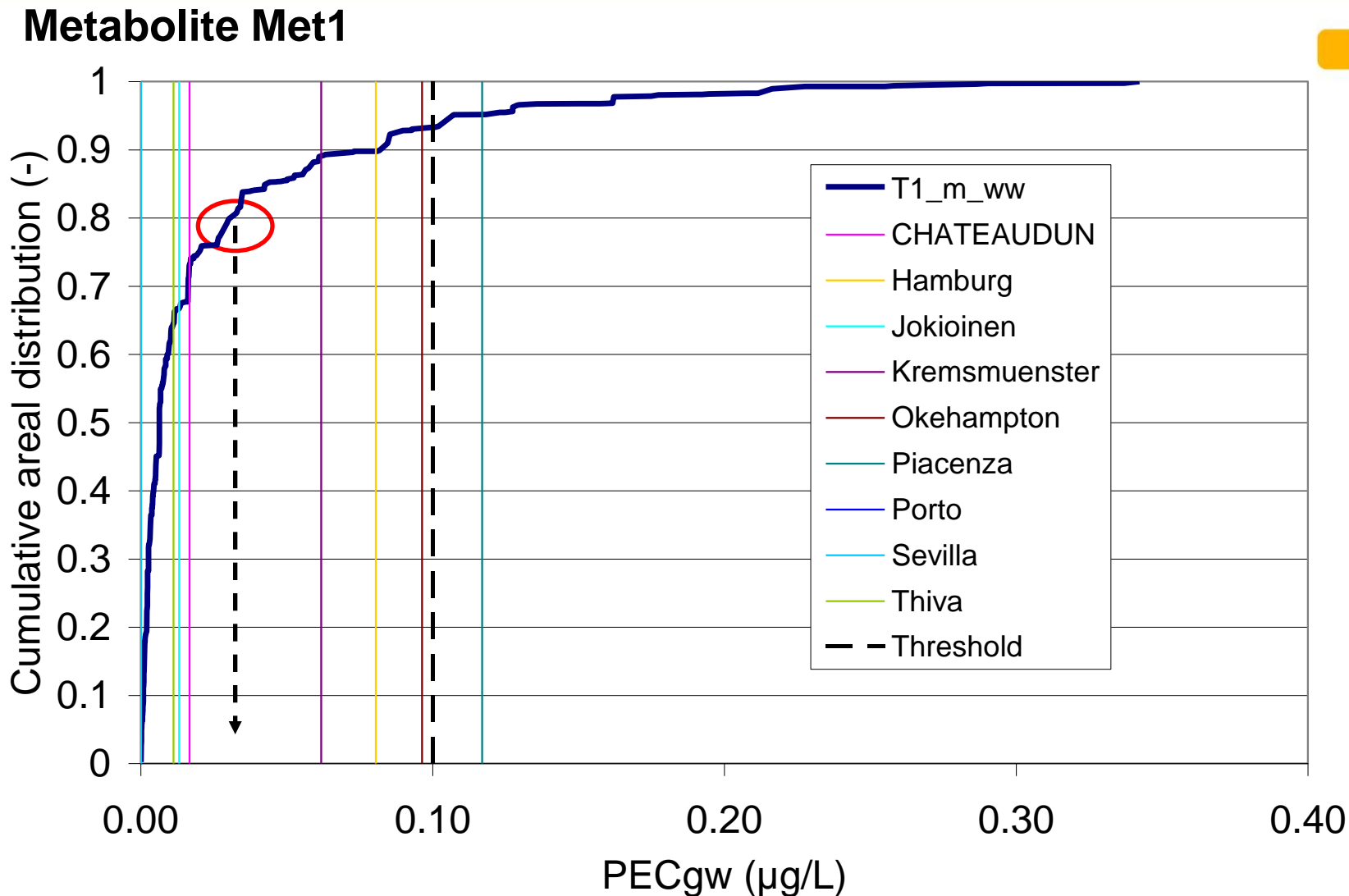


80<sup>th</sup> spatial percentile of FROGS scenarios = 12.8 µg/L → mitigation necessary

### Parent Test1

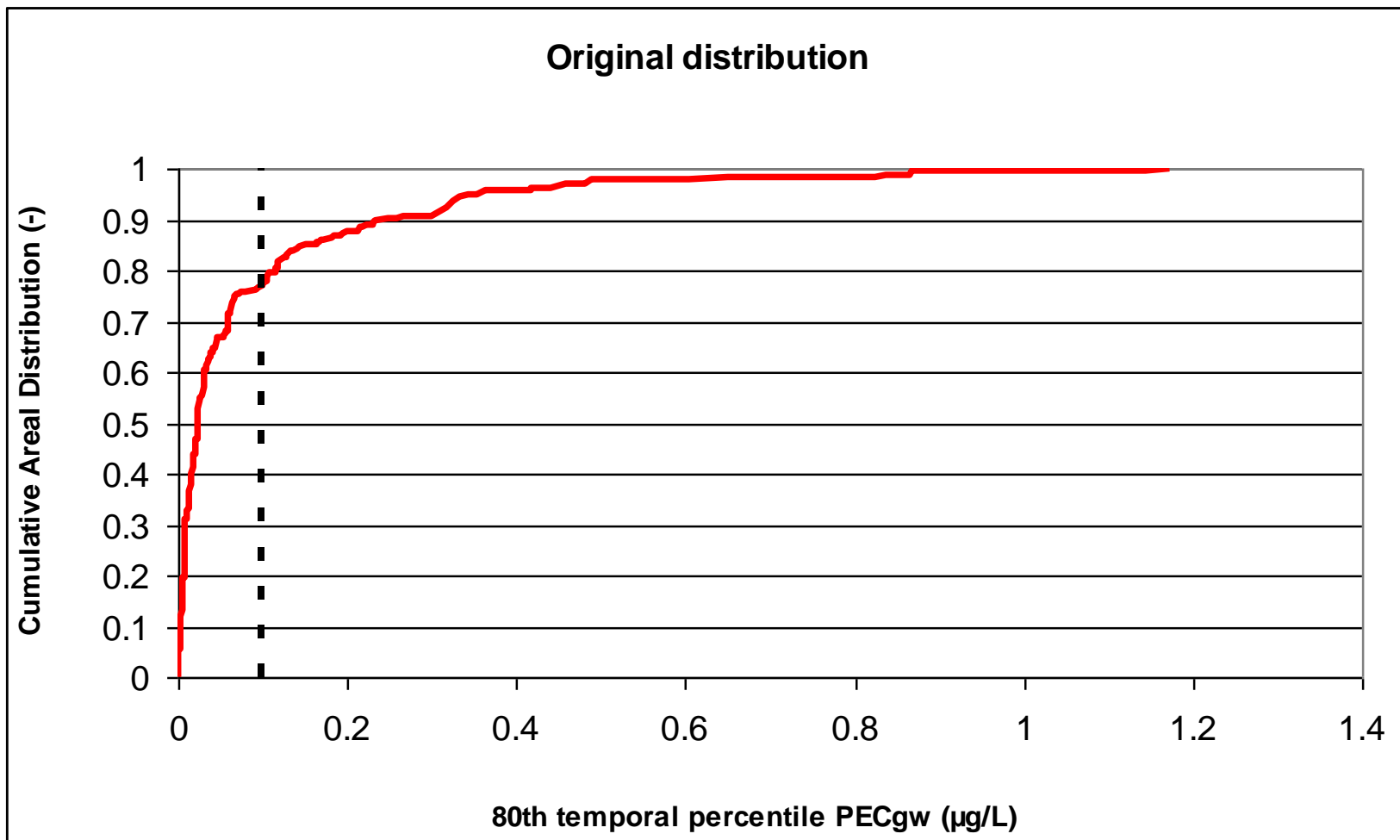


80<sup>th</sup> spatial percentile of FROGS scenarios = 0.113  $\mu\text{g/L}$  → mitigation necessary



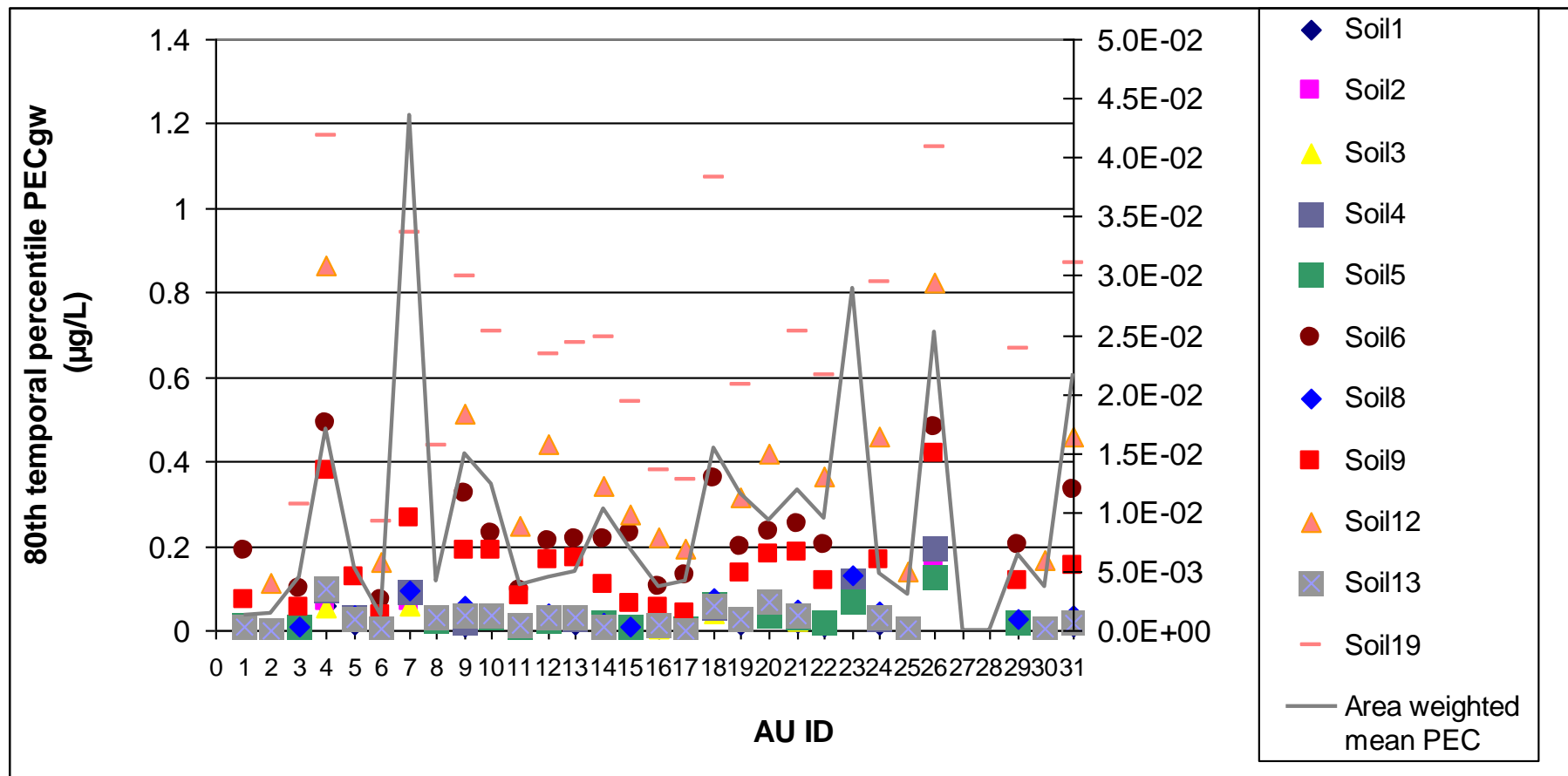
80<sup>th</sup> spatial percentile of FROGS scenarios < 0.1  $\mu\text{g/L}$

### Original Distribution (PEC = 0.113 $\mu\text{/L}$ )

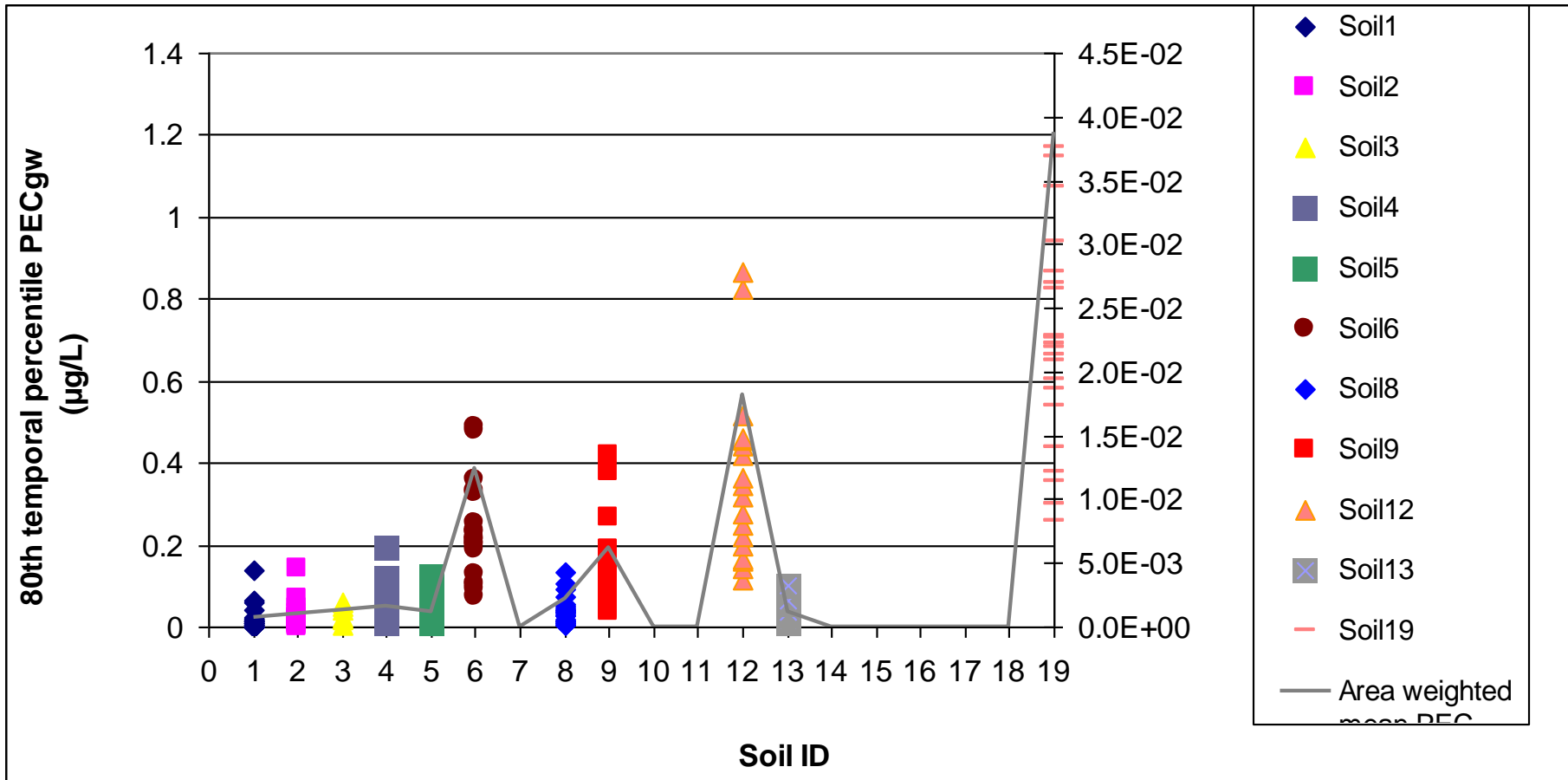




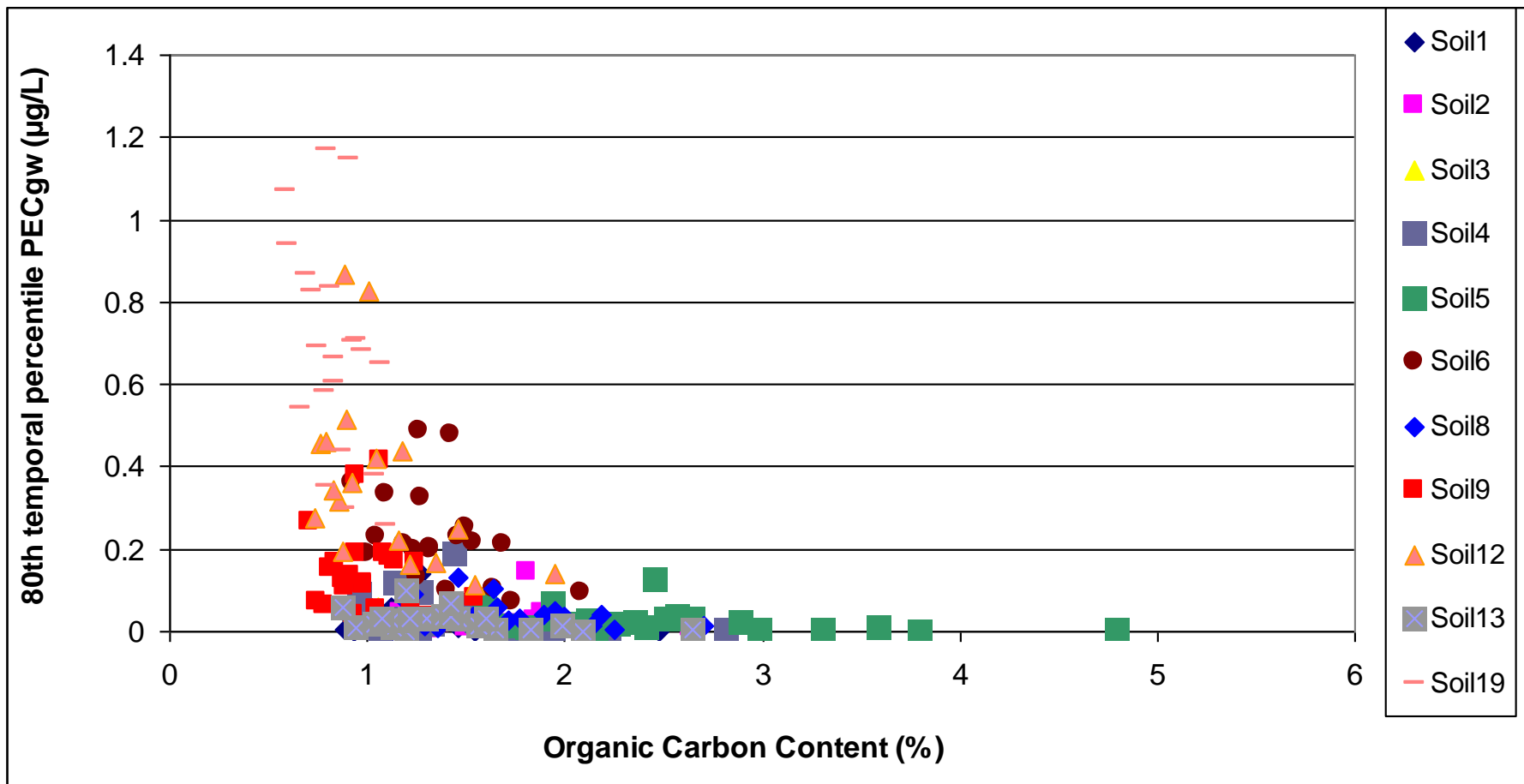
PECs sorted by Agronomic United → no clear pattern



### PECs sorted by Soil → PEC dependent on soil properties

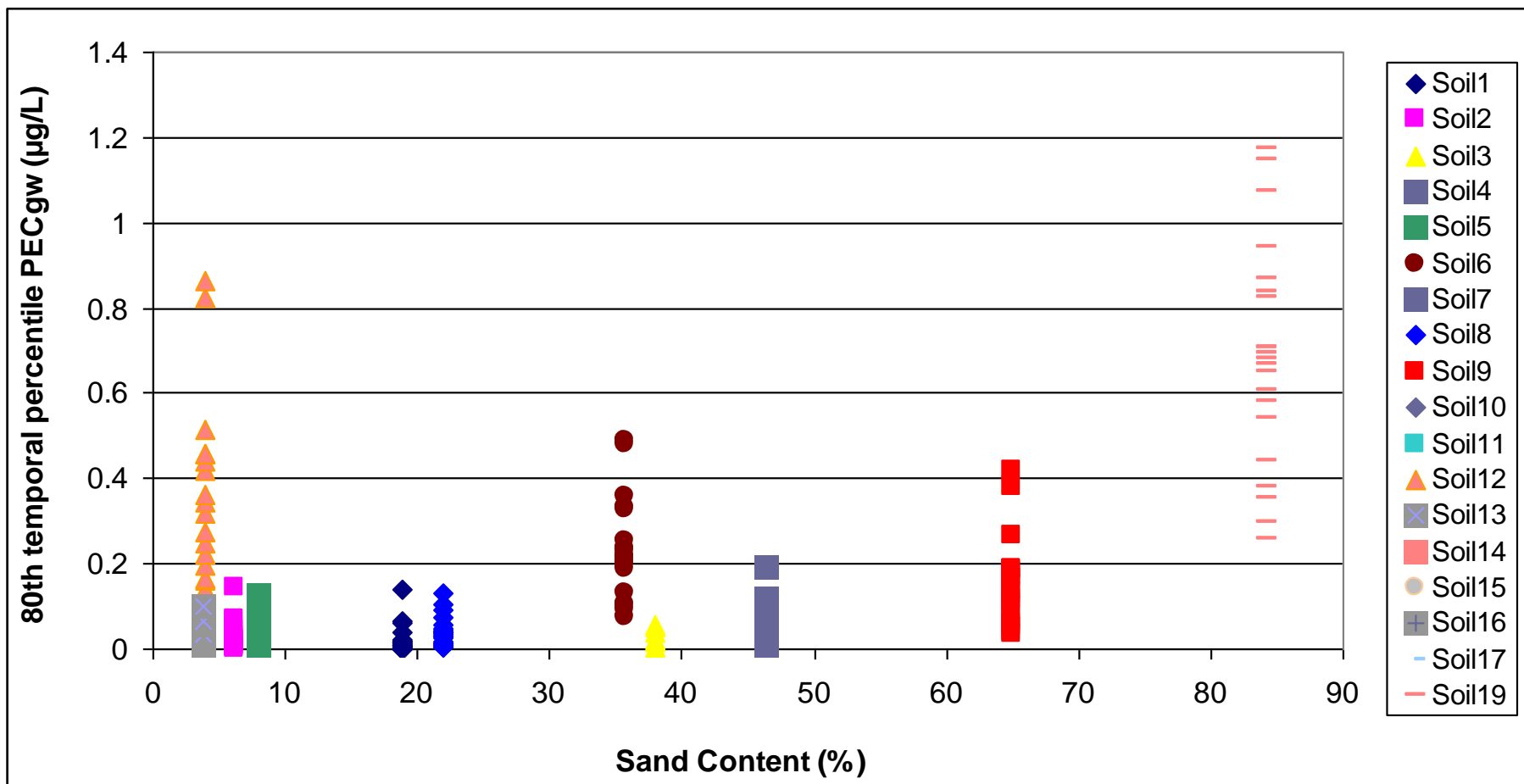


### PECs sorted by OC

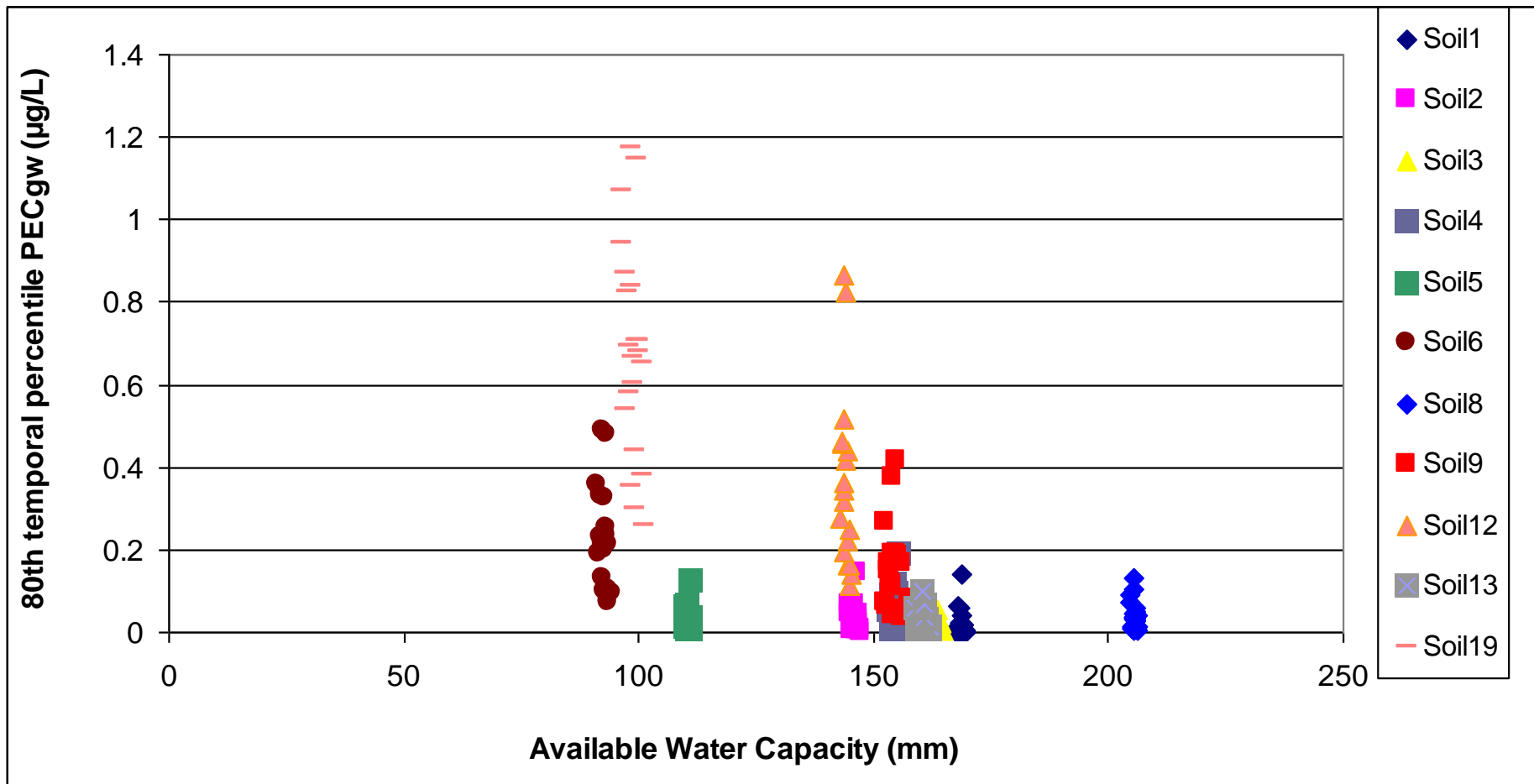




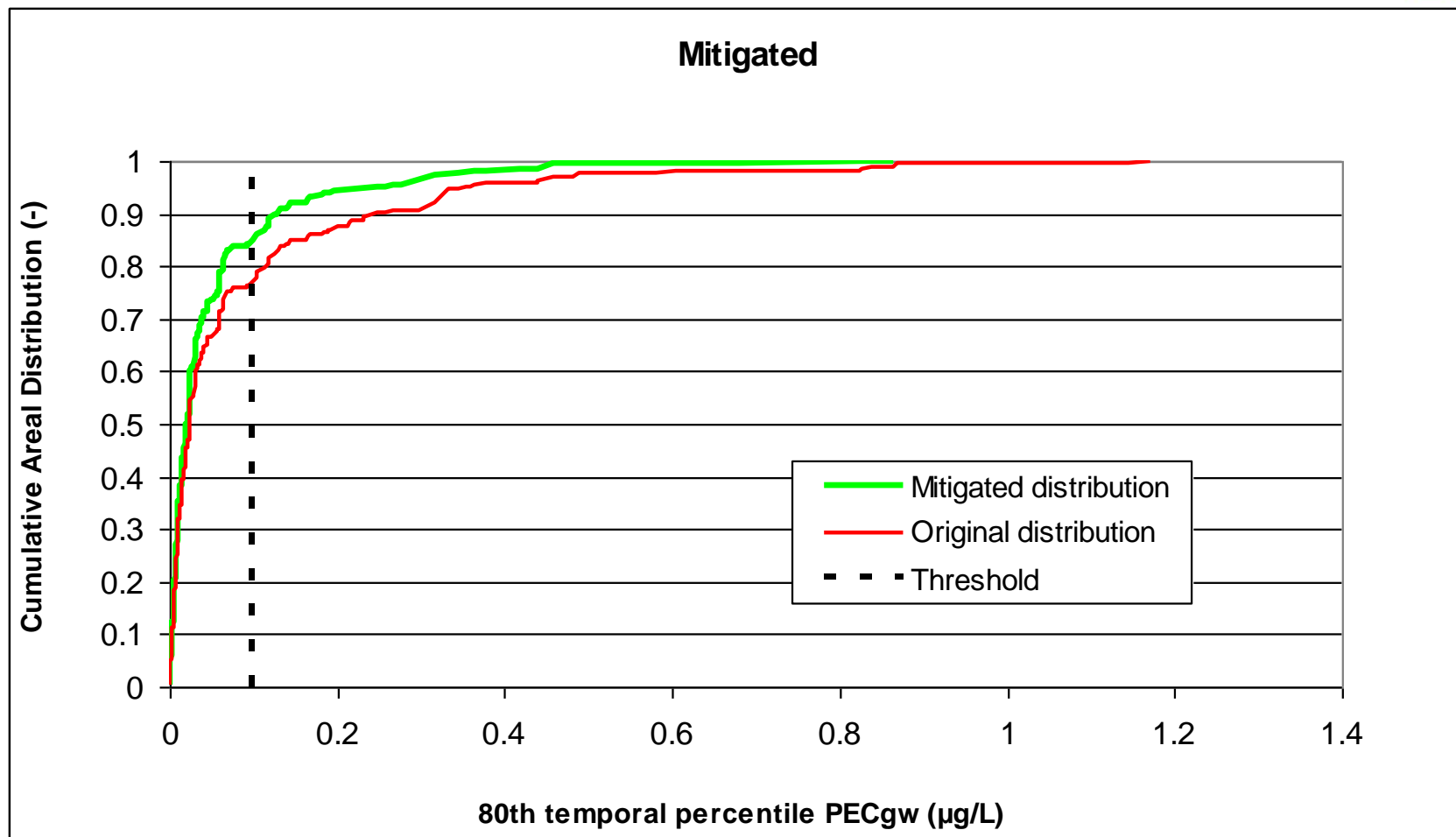
### PECs sorted by Sand content



### PECs sorted by Available Water Capacity



### Mitigated by AWC (<100 mm)



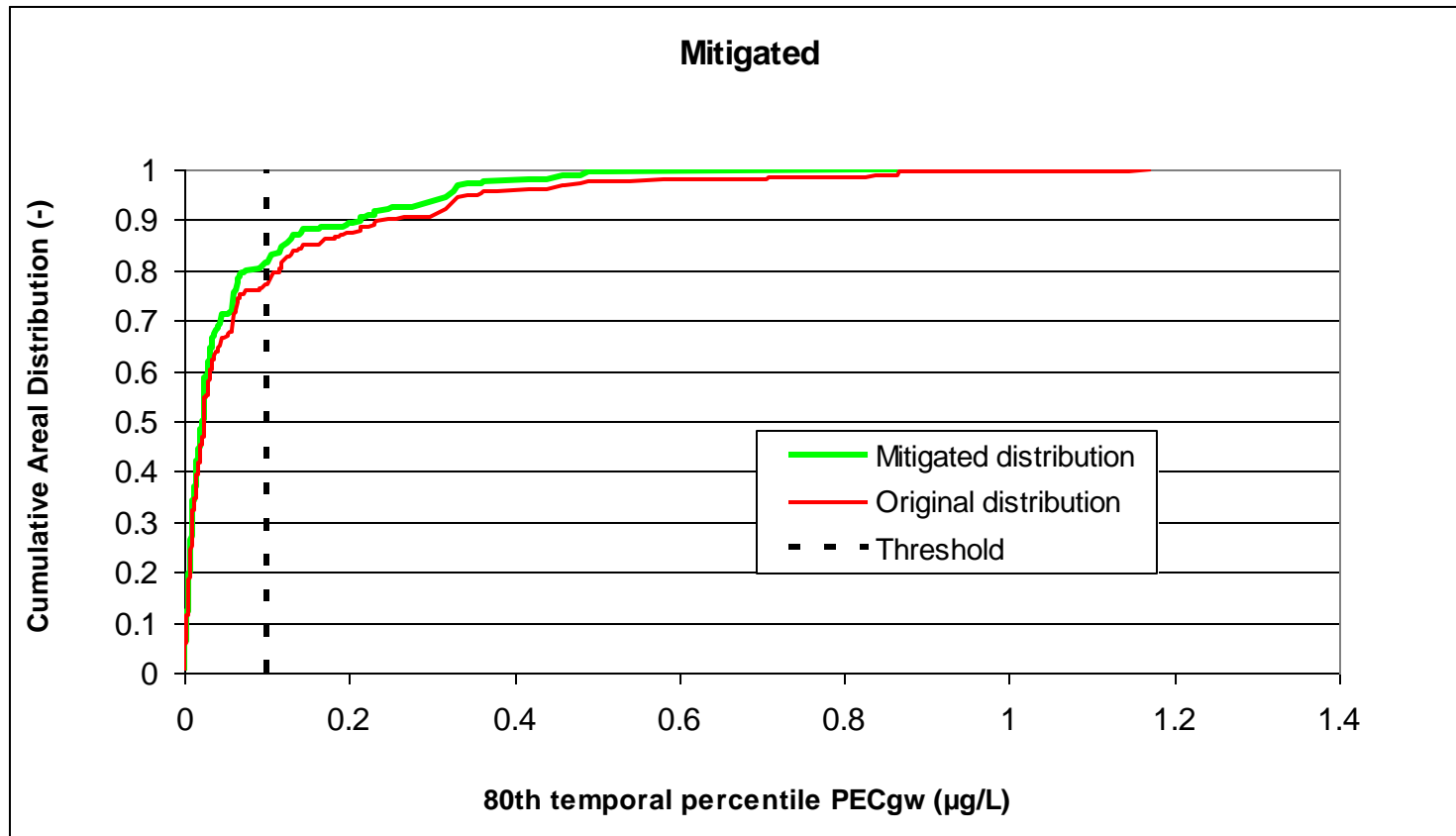
**PEC = 0.063  $\mu\text{g/L}$ ; Loss of area = 9.4%**



### Exercise 5:

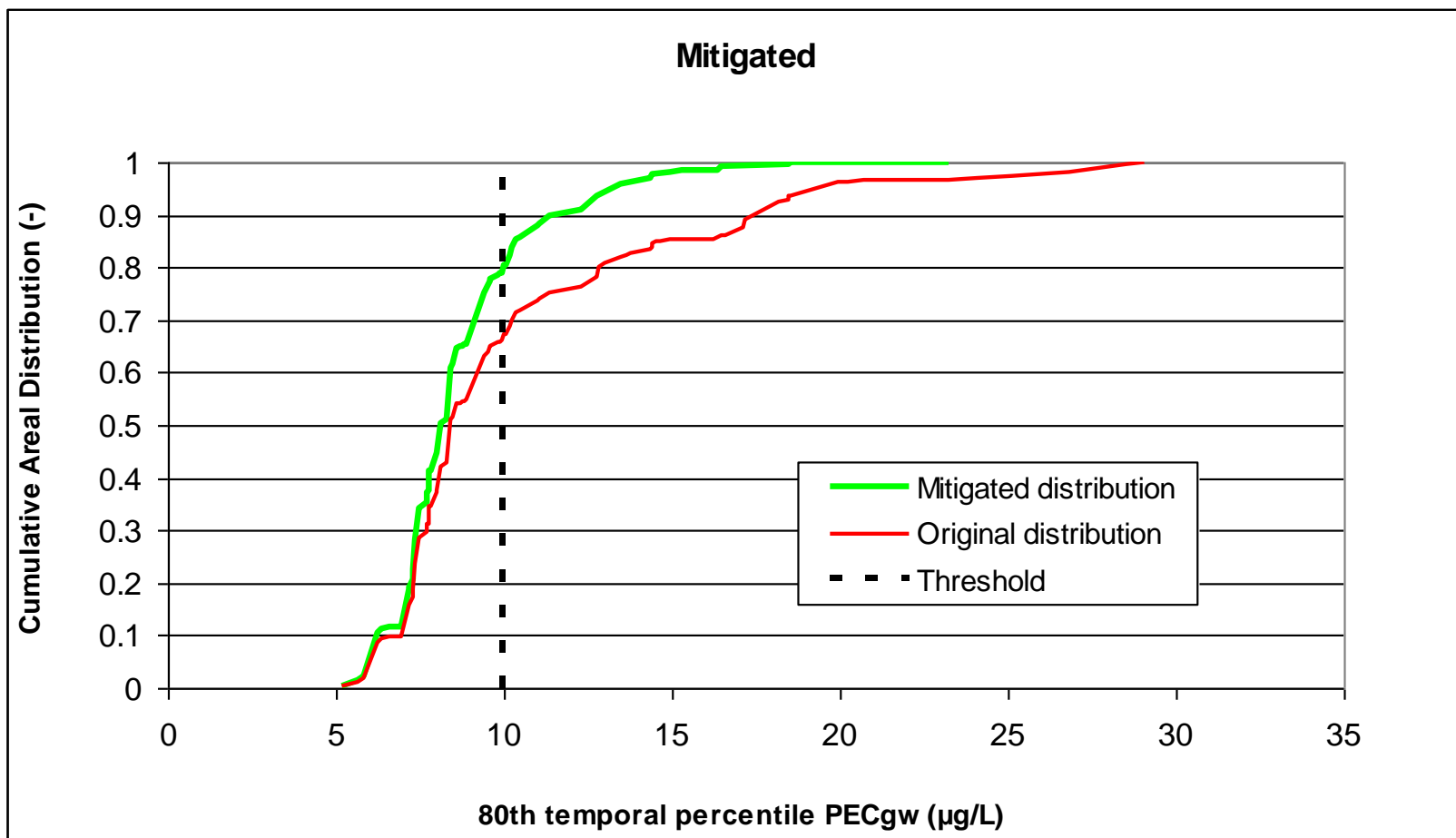
- Find complete „FROGS summary.txt“ files for both runs in folders „Exercise\\_SUBID\_frogs\_summary\FROGS summary.txt“. Import them each into a mitigation excel sheet.
- **Substance Test1**
  - Try further mitigation options
  - Is it possible to keep loss of application area < 9 %
- **Substance MetC**
  - Find different mitigation strategies leading to a PEC < 10µg/L?
  - Which one leads to a minimum loss of application area?

### Test1: Mitigated by Sand content (< 60%)



**PEC = 0.074 µg/L; Loss of area = 6.5%**

### MetC: Mitigated by OC (< 0.9%) or AWC (< 100 mm)



**PEC = 9.971 µg/L; Loss of area = 16.3%**



Thank you very much for your kind attention