4. DEMO AND EXERCISES

FROGS (French Refinement Of Groundwater Scenarios)
UIPP Training

Paris, 16 November 2011

UIPP Environmental Methodology Working Group

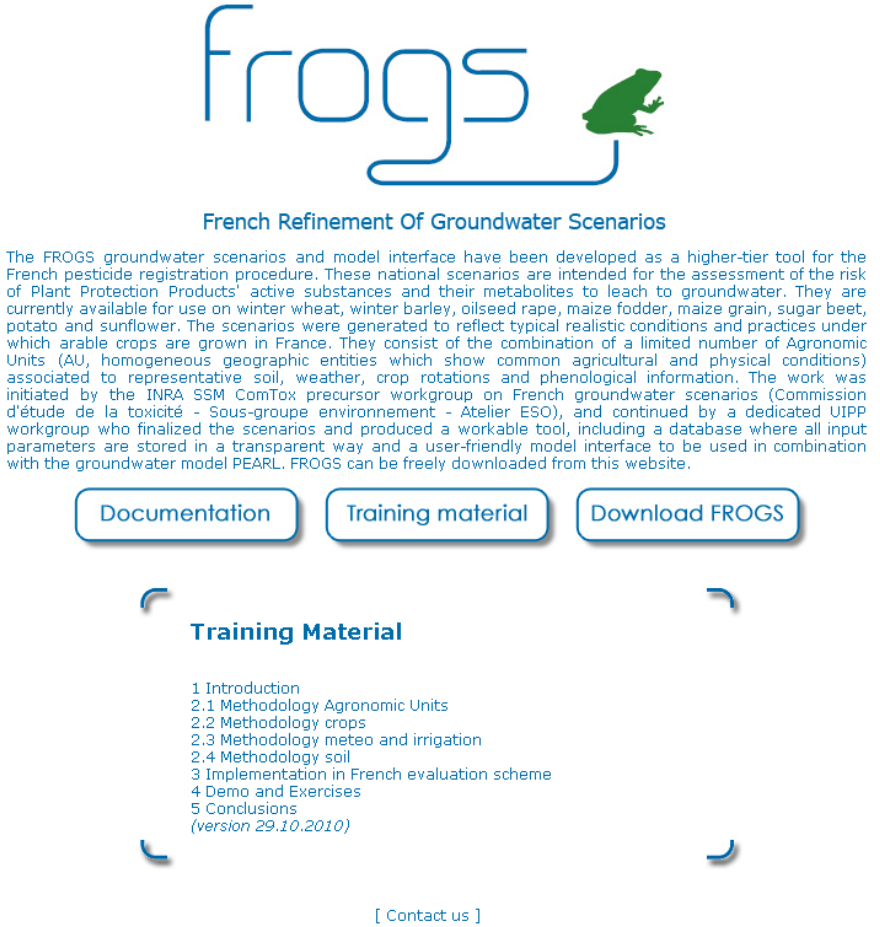
Outline

1. **Introduction to FROGS GUI**
   - Create FROGS project
   - Run and Evaluate FROGS

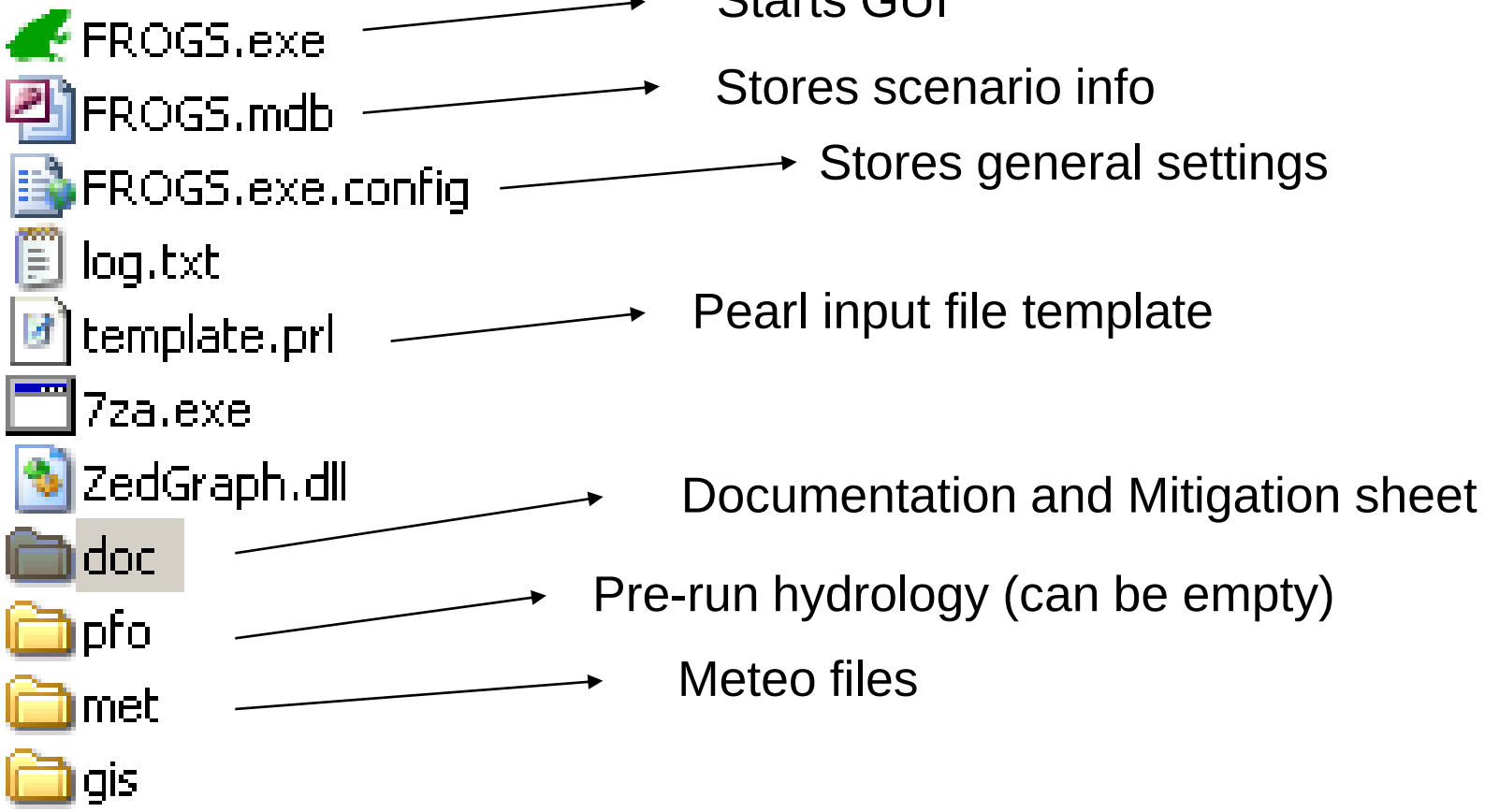
2. **FROGS Mitigation Sheet**

Download

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



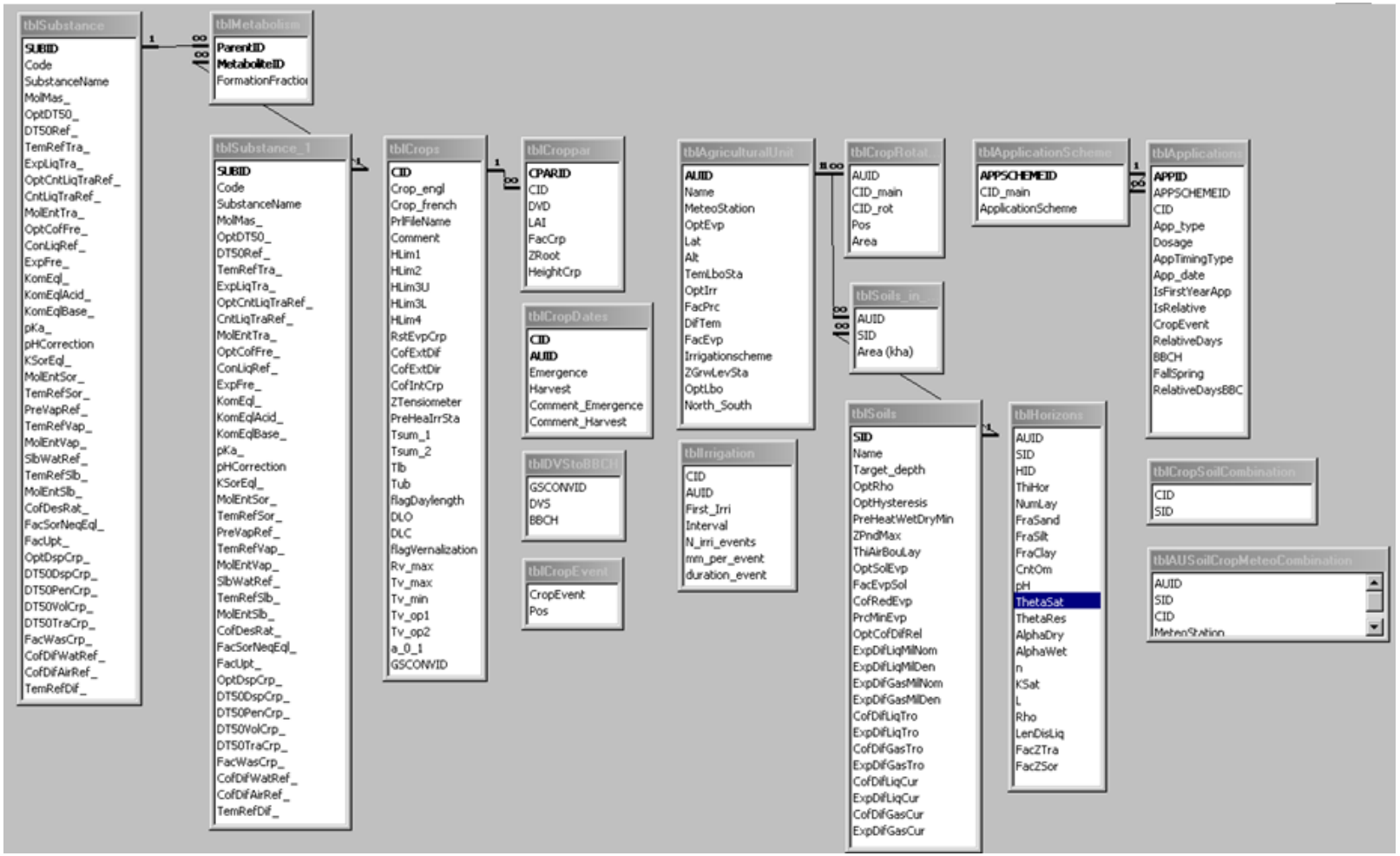
Download



! pearlmodel.exe/swap209e.exe have to be available on your computer !

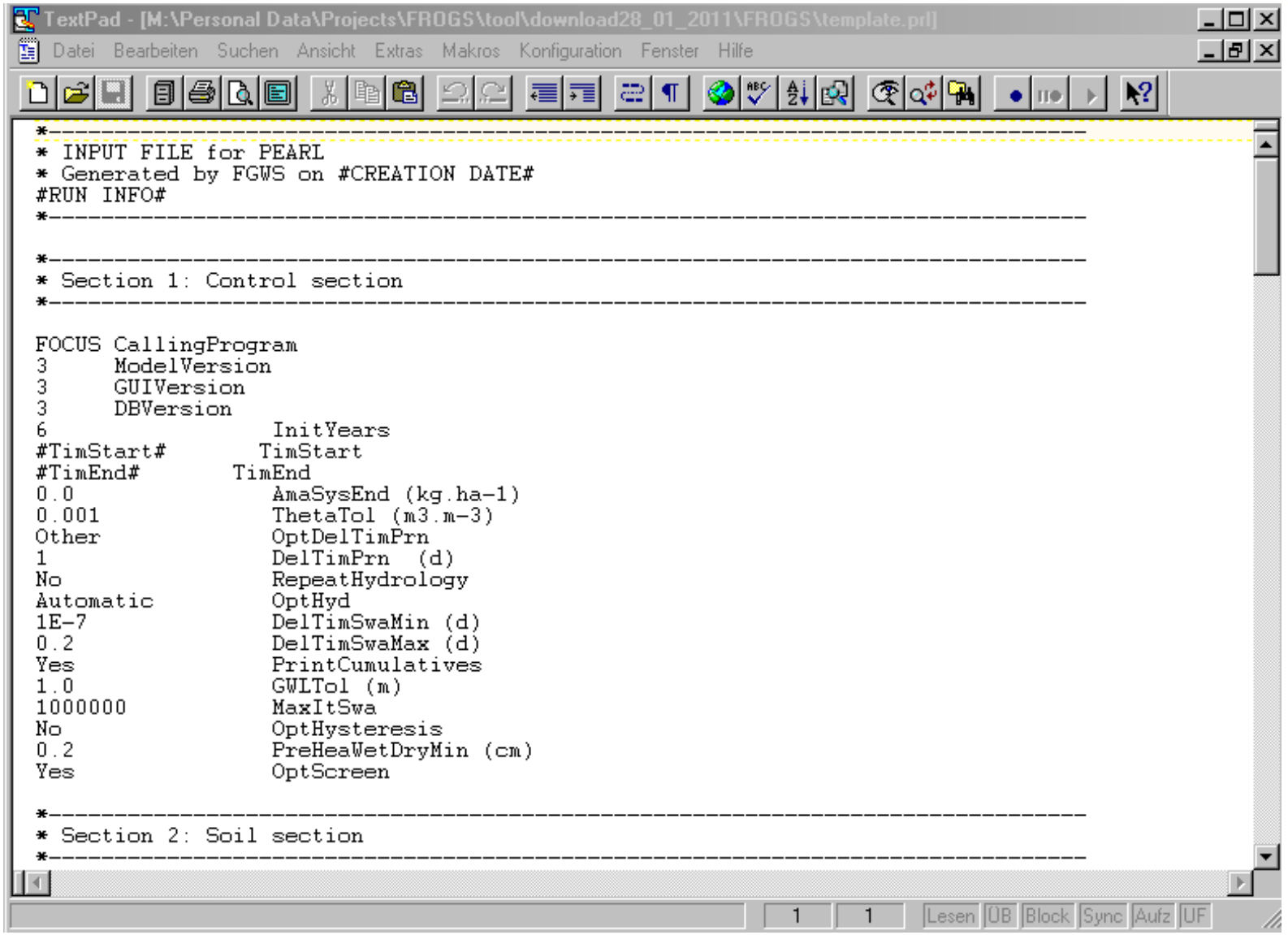
! No PEARL installation necessary !

FROGS database (*.mdb)



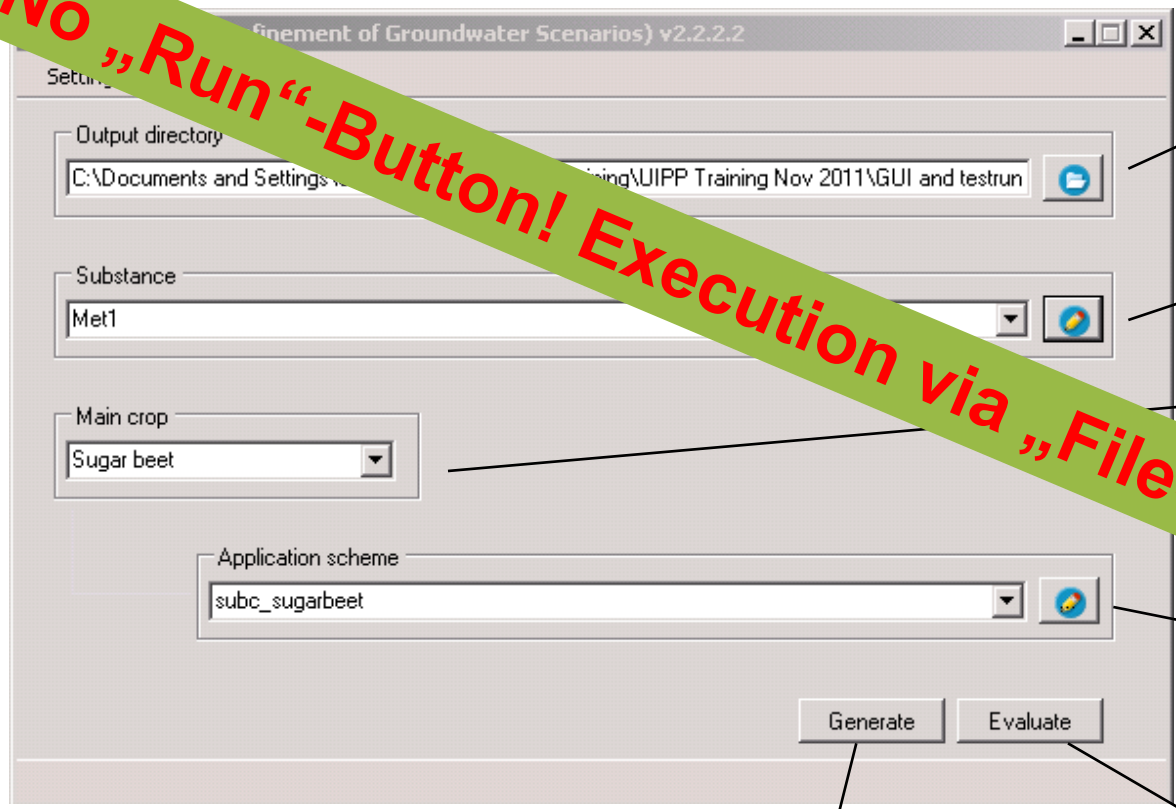
French Refinement Of Groundwater Scenarios

FROGS template file (template.prl)



Start Screen

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

Definition Application Scheme

Generates Input files in working directory

Evaluates output files from working directory

Settings

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

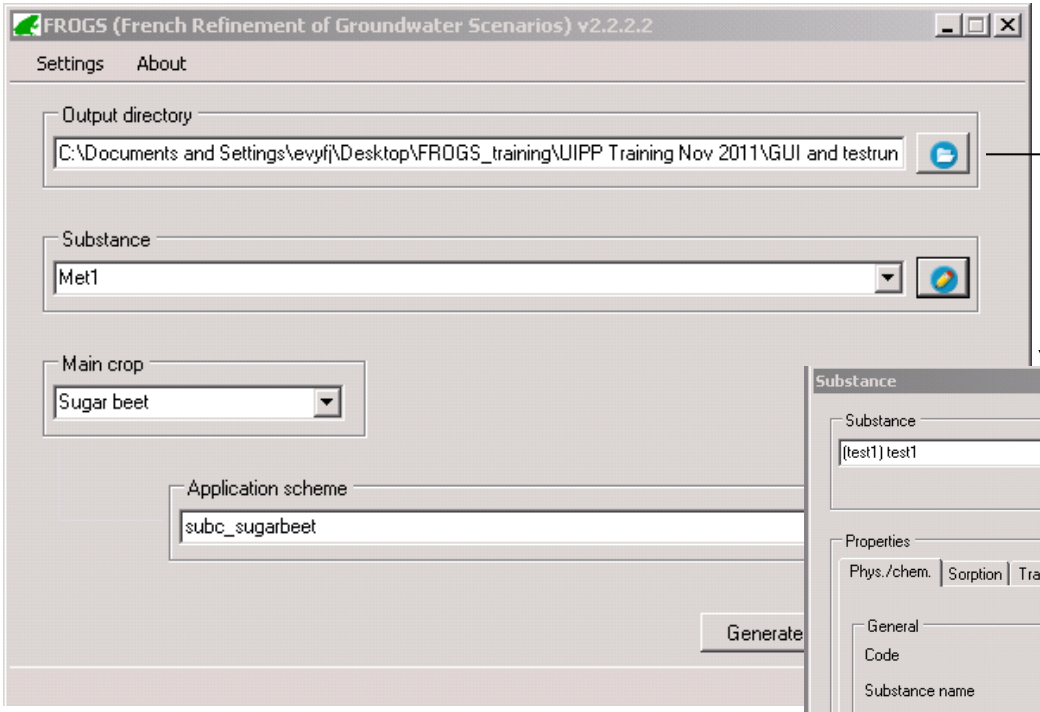
Location of pre-run hydrology files (has to be specified even if *.pfo files are not used)

Exercise 1: Initial Settings

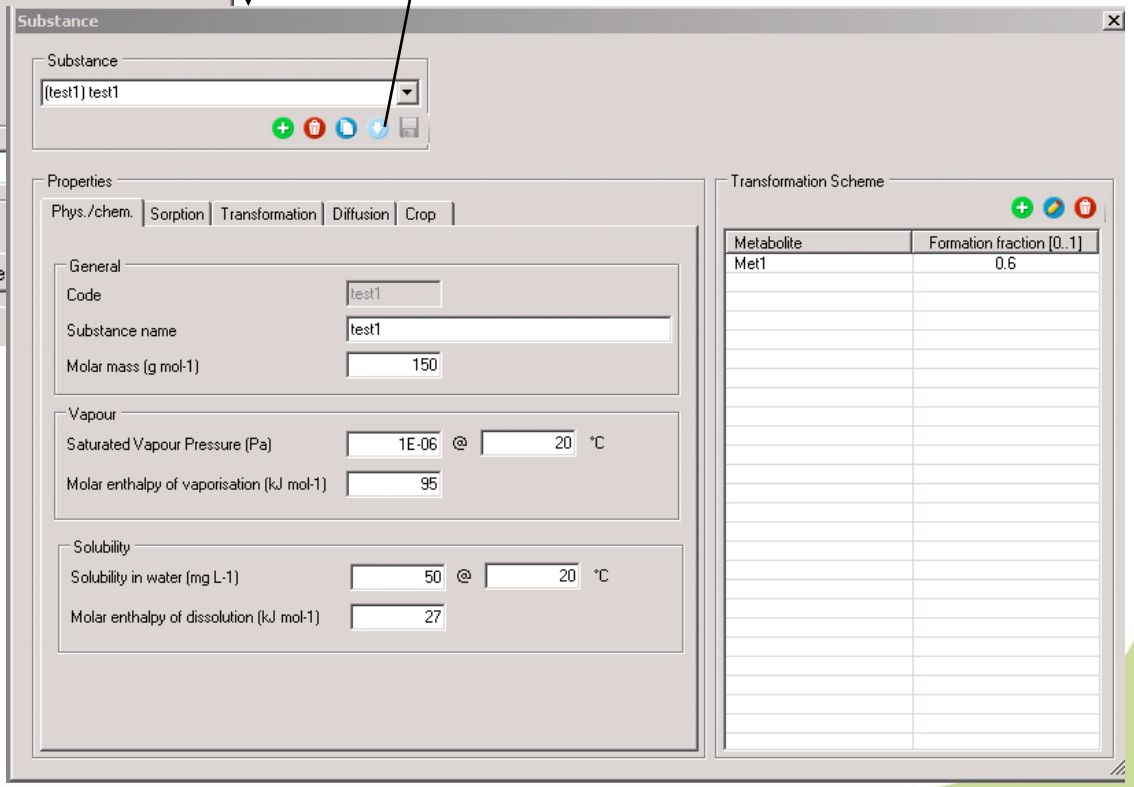
Exercise 1:

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

Substance definition



Option to import existing *.prl files



Formation fractions are not imported ➔ enter manually after import

Exercise 2: Substance Definition

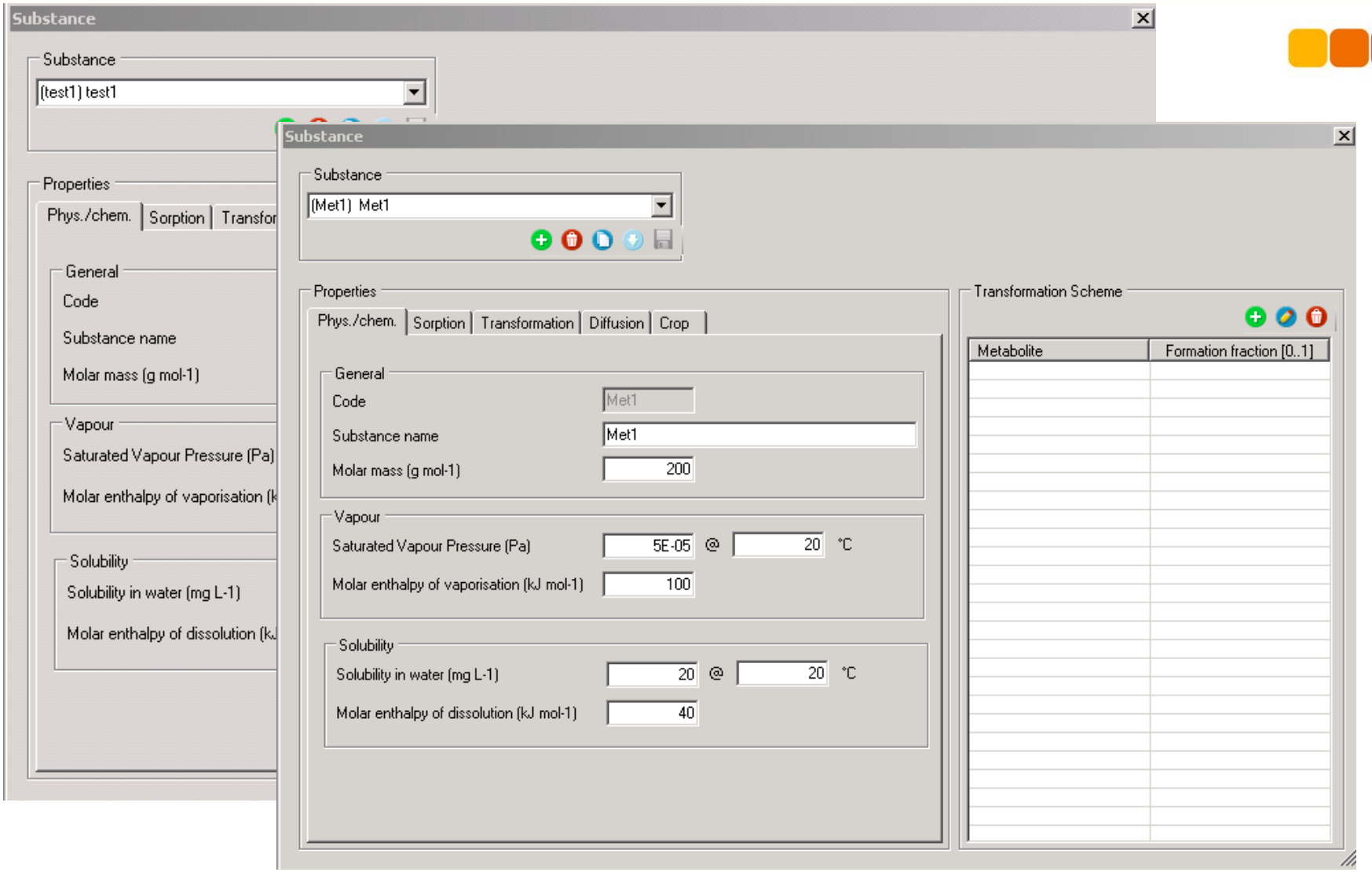
Exercise 2:

- 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

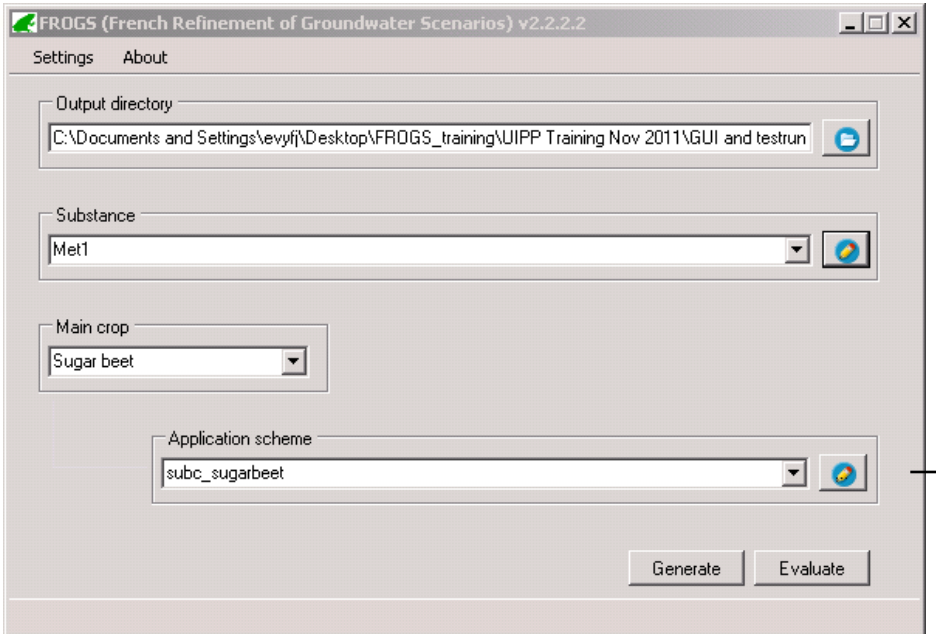
Exercise 2: Substance Definition

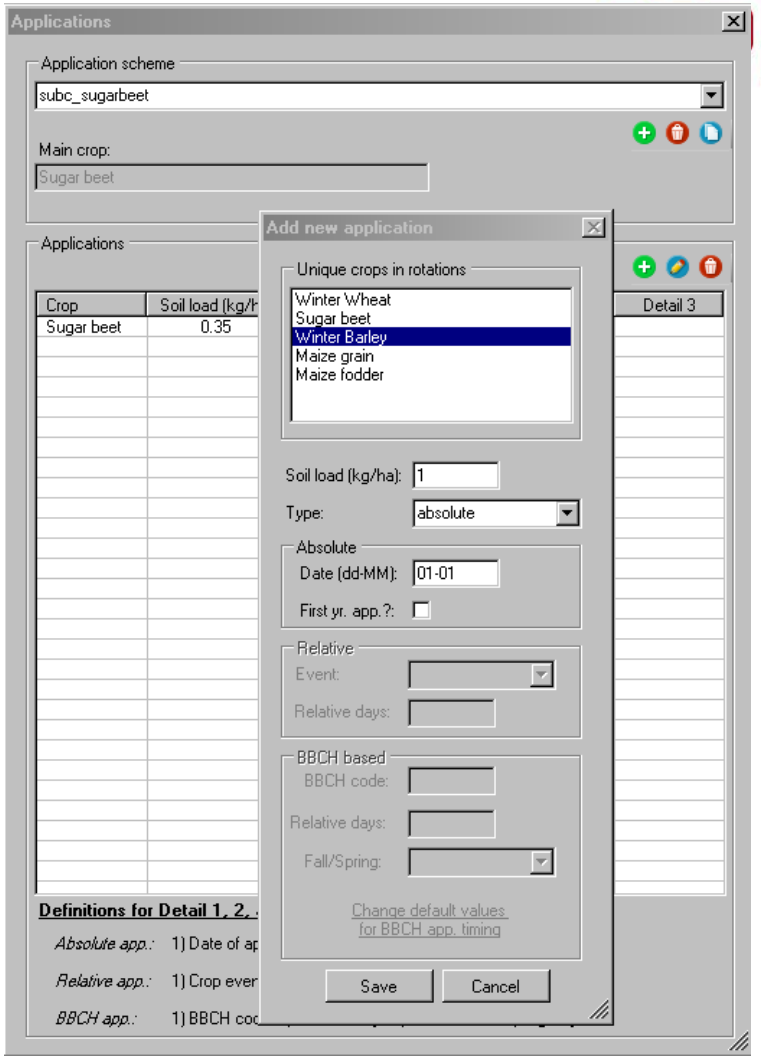
Parameter	SubC		Test1	
	Parent	Metabolite	Parent	Metabolite
Formation fraction	-	0.71	-	0.6
DT50 (d)	20	100	80	30
Kom (L/kg)	100	30	90	120
1/n	0.9	0.9	0.9	0.9
Solubility (mg/L)	50	90	50	20
Molar weight (g/mol)	200	150	150	200
Vapour pressure (Pa)	1E-10	1E-10	1E-6	5E-5
Mol. Enth. of Vapor. (kJ/mol)	95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

Exercise 2: Substance Definition



Application Scheme

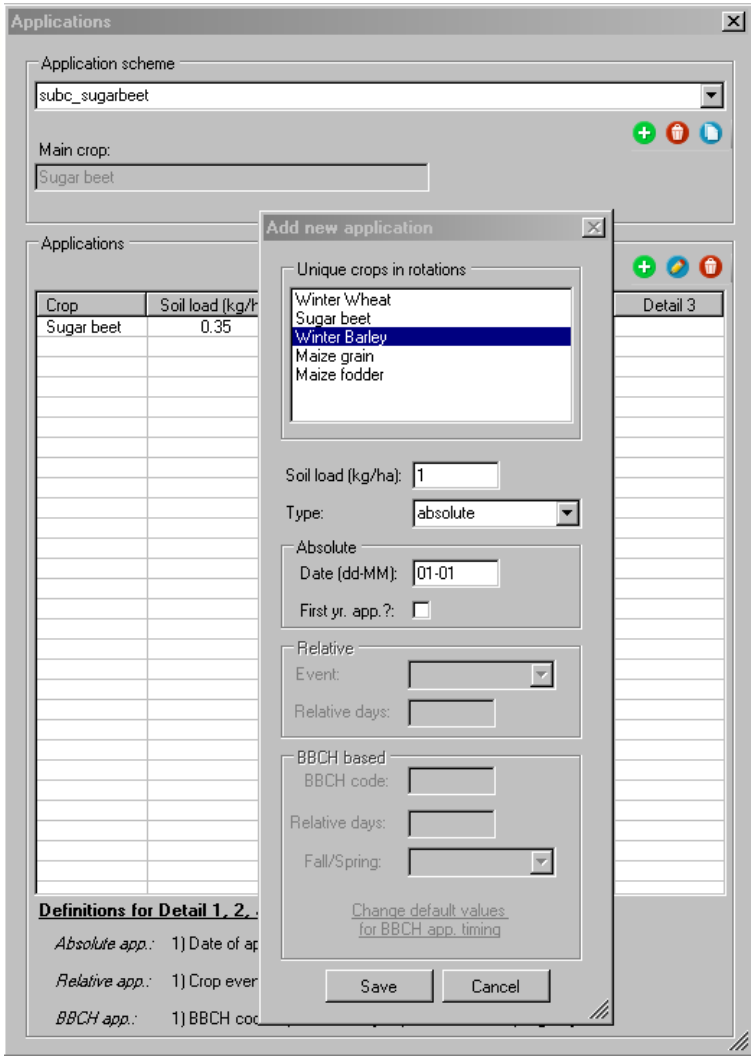




Each Application scheme consists of 1 – X applications

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

Application Scheme



- 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: Application scheme

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: Application scheme

Exercise 3 (continued):

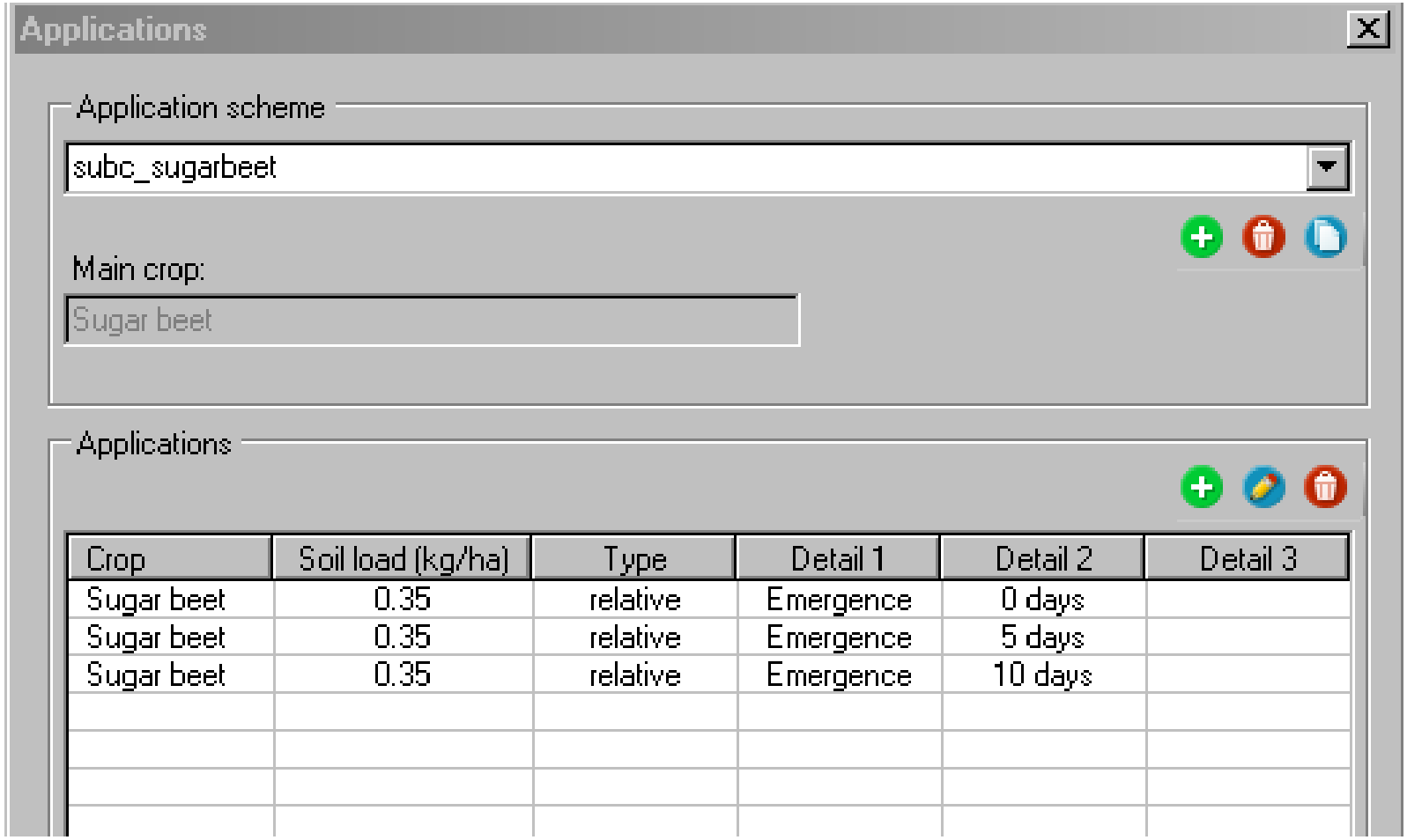
If you still have time left…

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 1st December (0.15 kg/ha)
- **winter barley**
  - 3 applications at BBCH 39-69 with 10 days interval (each 0.1 kg/ha)

Exercise 3: Application scheme

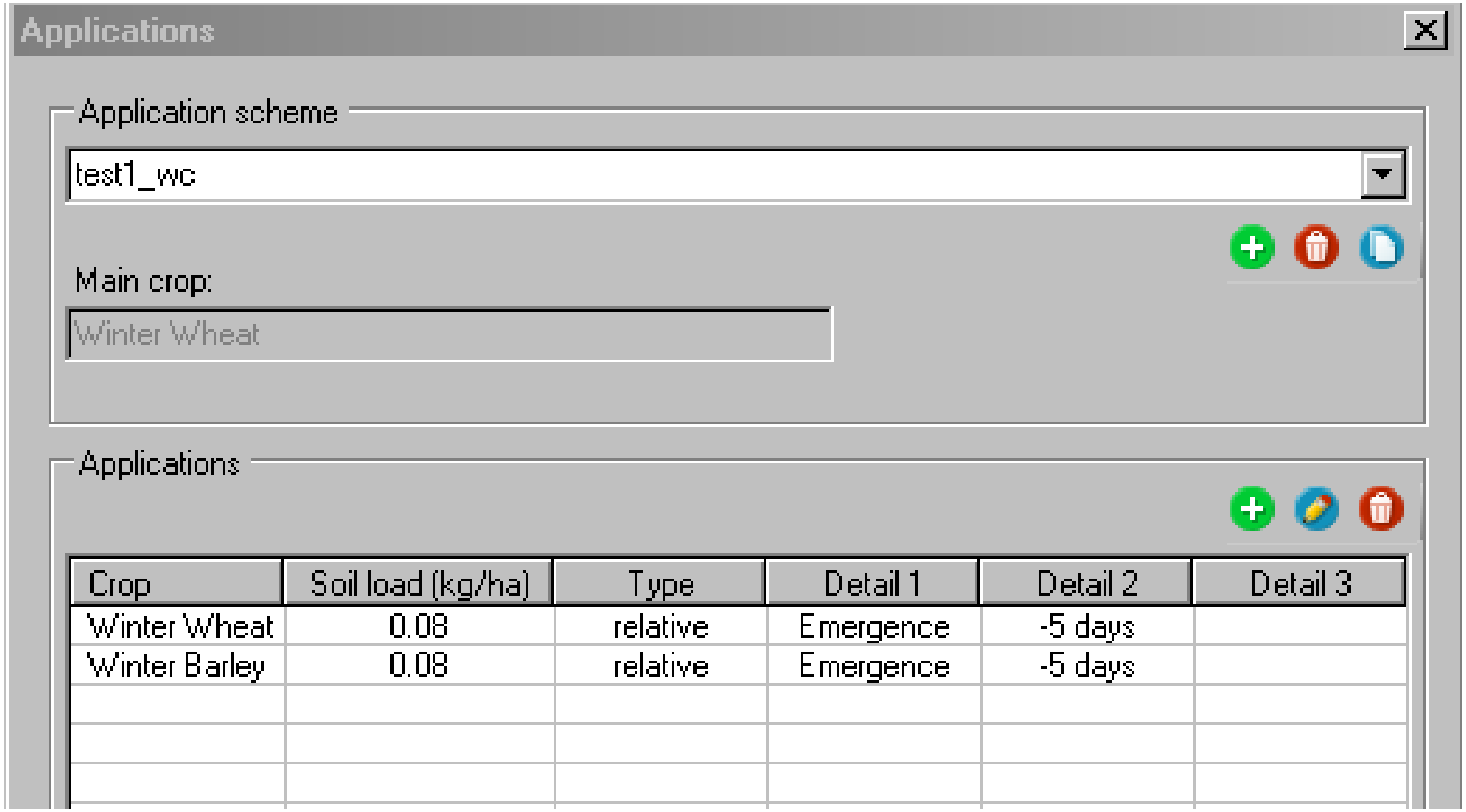
„subC_Sugarbeet“



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	

Exercise 3: Application scheme

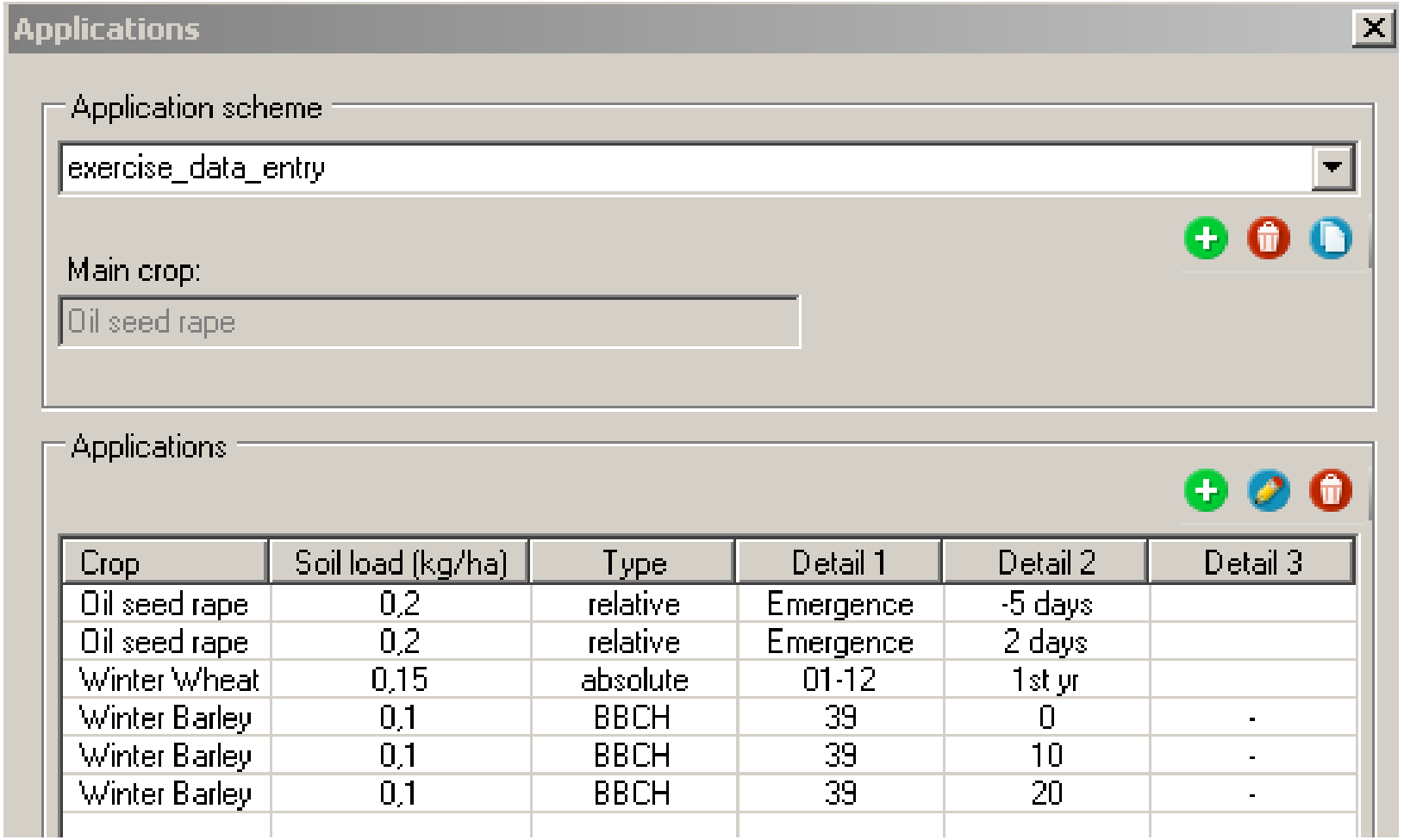
„test1_wc“



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	

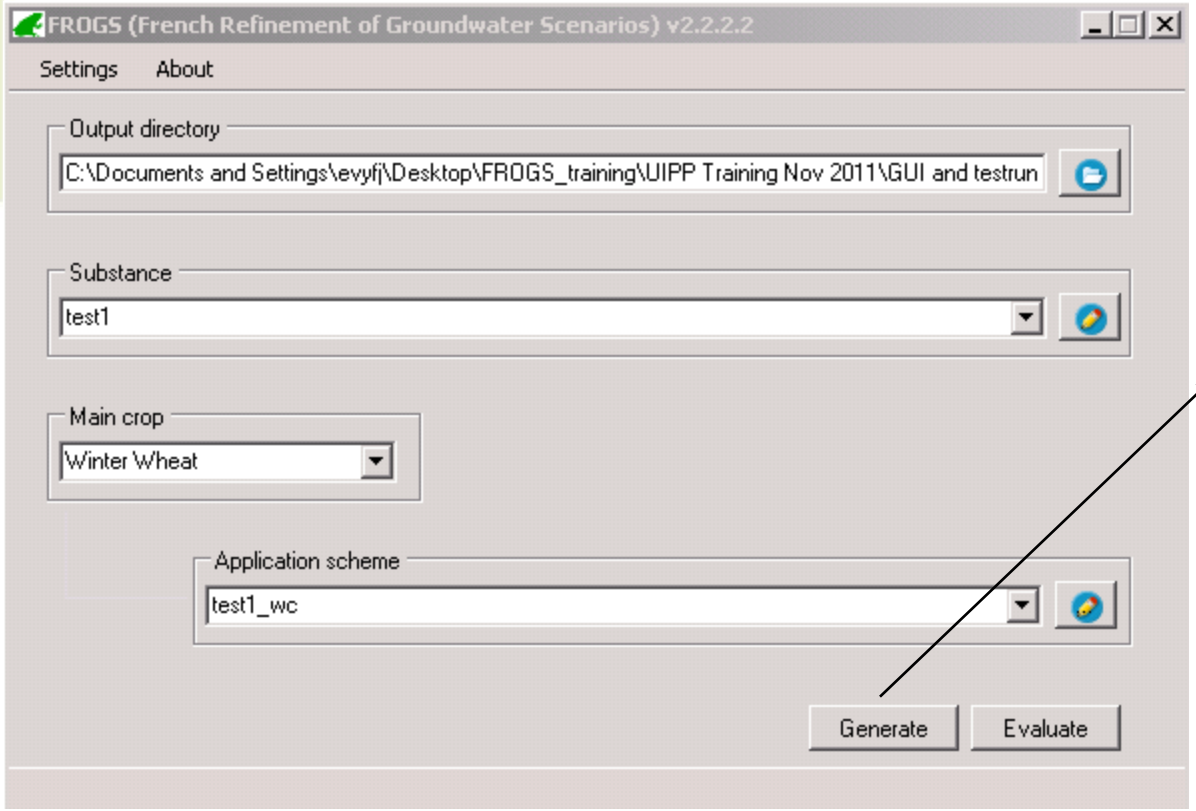
Exercise 3: Application scheme

„exercise_data_entry“



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	-

Generate Input

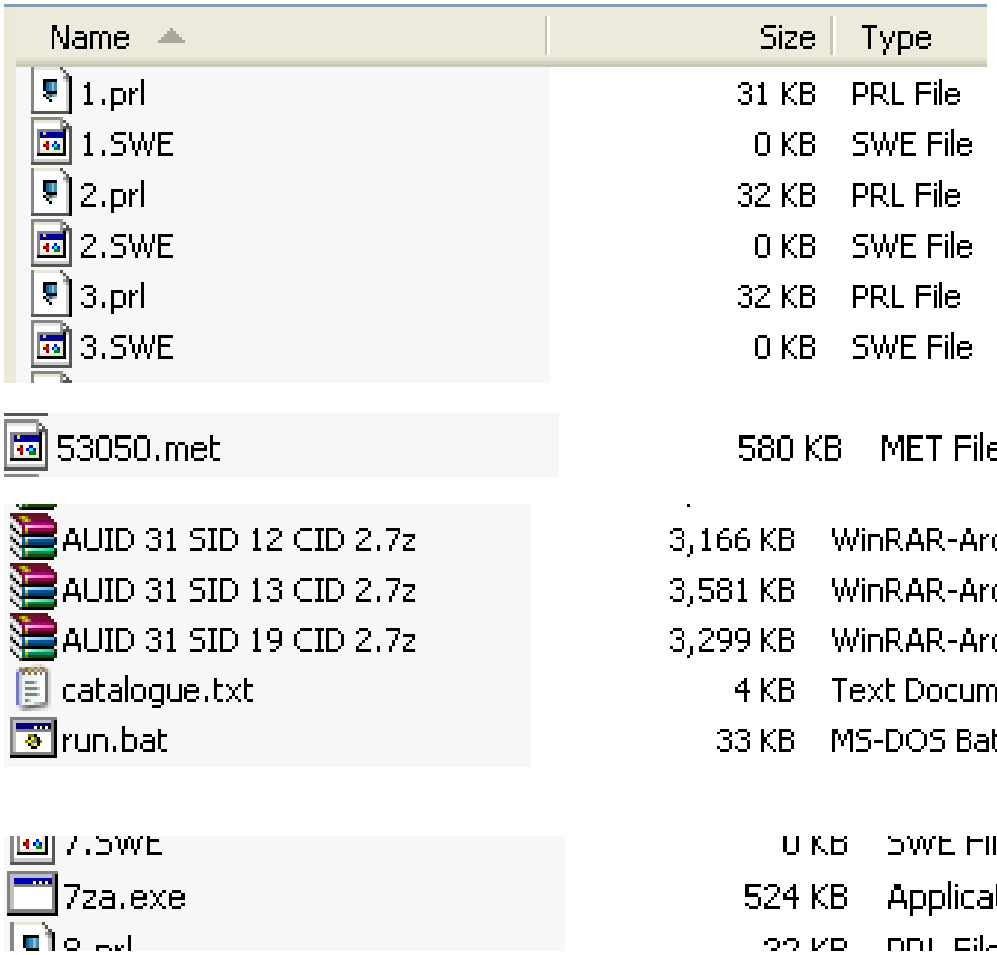


After defining all details click „Generate“ to generate all input.

➔ Allows modification/distribution of runs before execution

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

Input files



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

Meteo files

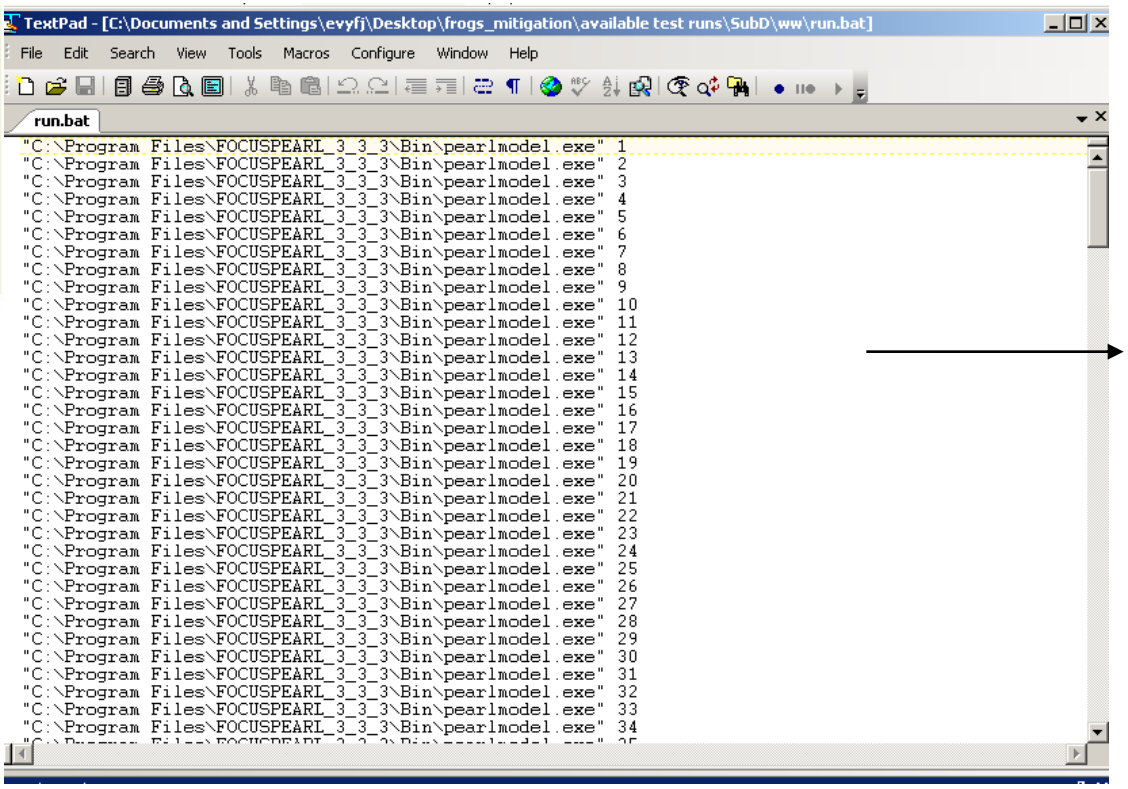
Zipped *.pfo files

Summary of all runs

Batch file to run FROGS

Program to unzip *.pfo files

Run.bat



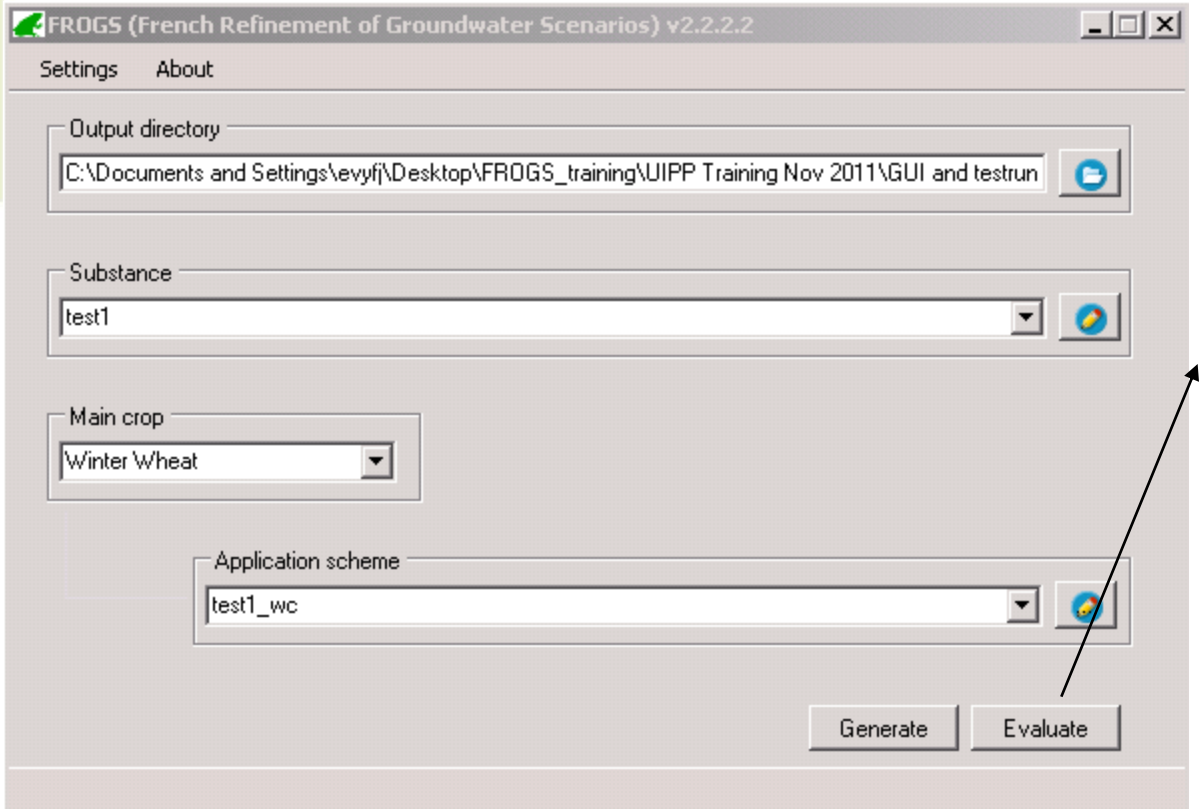
No *.pfo files available ➔ SWAP will be executed

```
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

Evaluate



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”

French Refinement Of Groundwater Scenarios

FROGS summary.txt

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

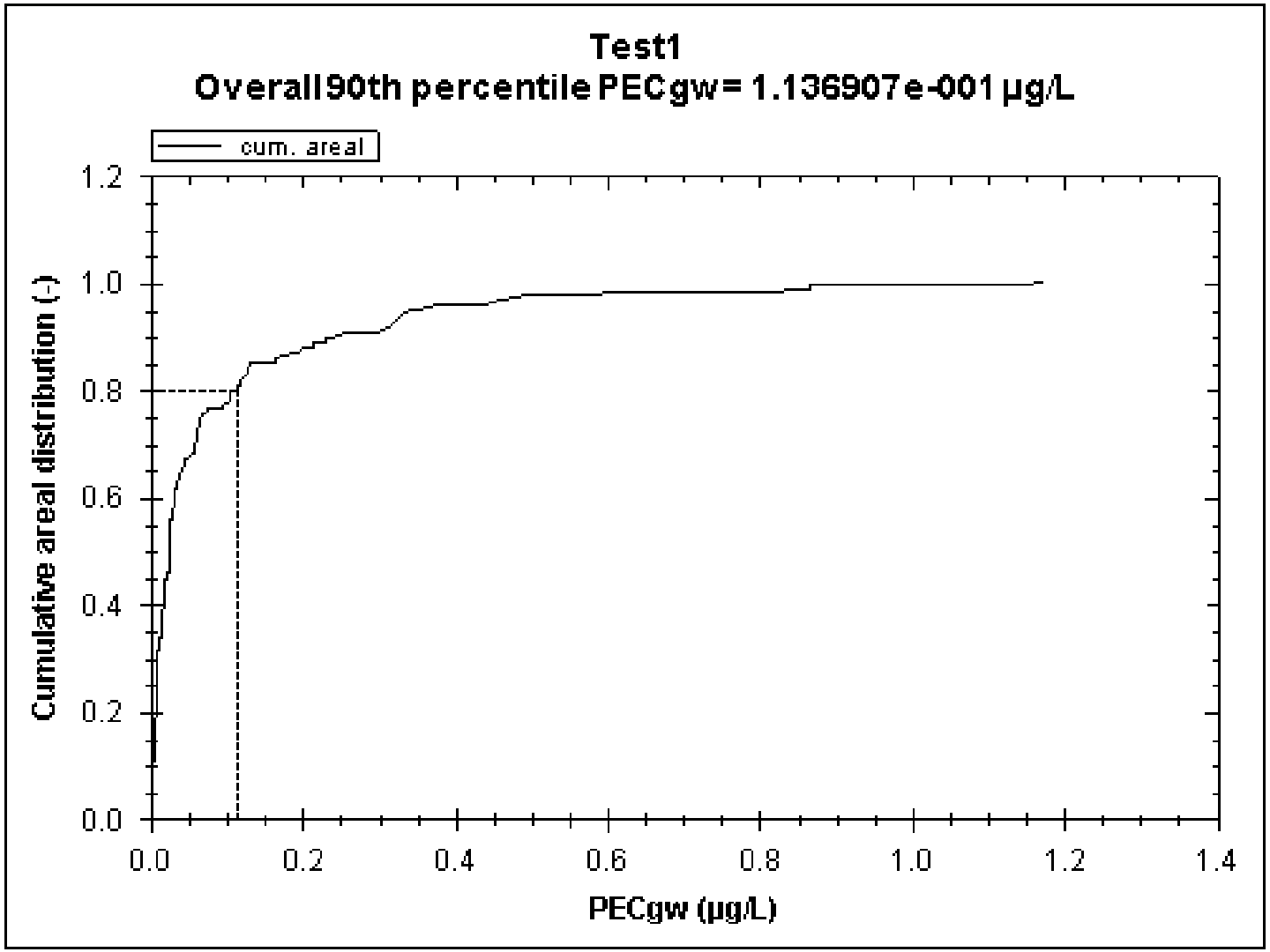
```
**** Compounds
                    SubC              MET-C
MolMas_*            200               150               (g.mol-1)     Molar mass [10|10000]
OptDT50_*           Input             Input                           Option for DT50: Input or Calculate
DT50Ref_*           20                100               (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]
SlbWatRef_*         50                90                (mg.L-1)      Solubility in water [1e-9|1e6]
TemRefSlb_*         20                20                (C)           .. measured at [0|40]
MolEntSlb_*         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
            (kg/ha)
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        571     SBEET-WWHEAT-WWHEAT     2       SubC    4.337176878438 47E-10   1999
1       4       Bordure Nord - Picardie - Normandie     1       Luvisol 3 >80 cm        571     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



80th spatial percentile of FROGS scenarios = 0.113 µg/L ➔ mitigation necessary

Exercise 4: Run FROGS

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

Exercise 4: Run FROGS

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

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 !

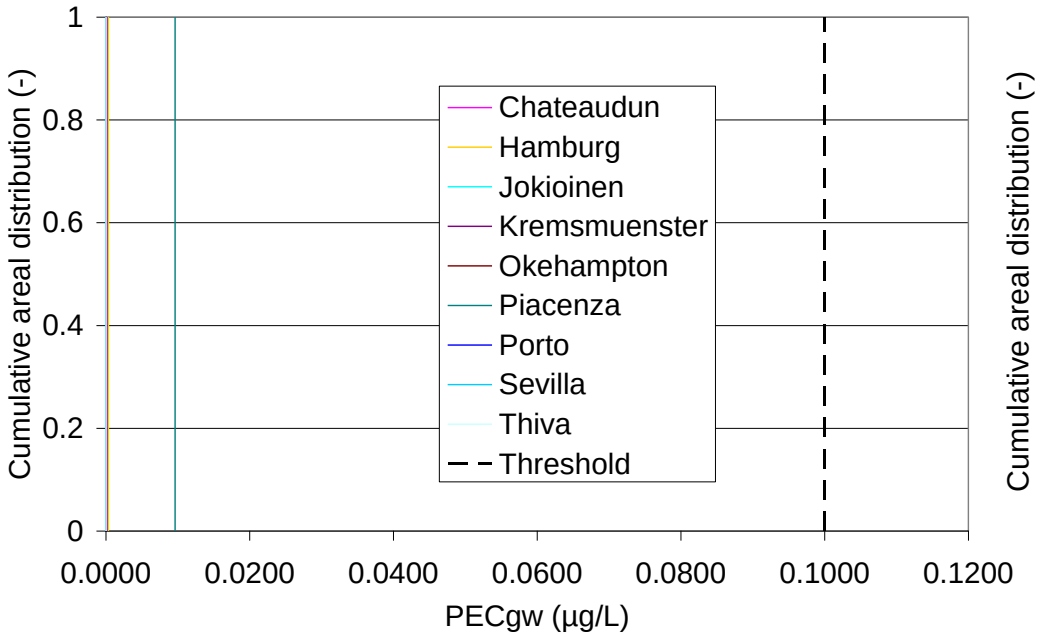
➔ Use Excel-Sheet „FROGS template mitigation.xls“ to check and apply mitigation options

Mitigation: FOCUS Results

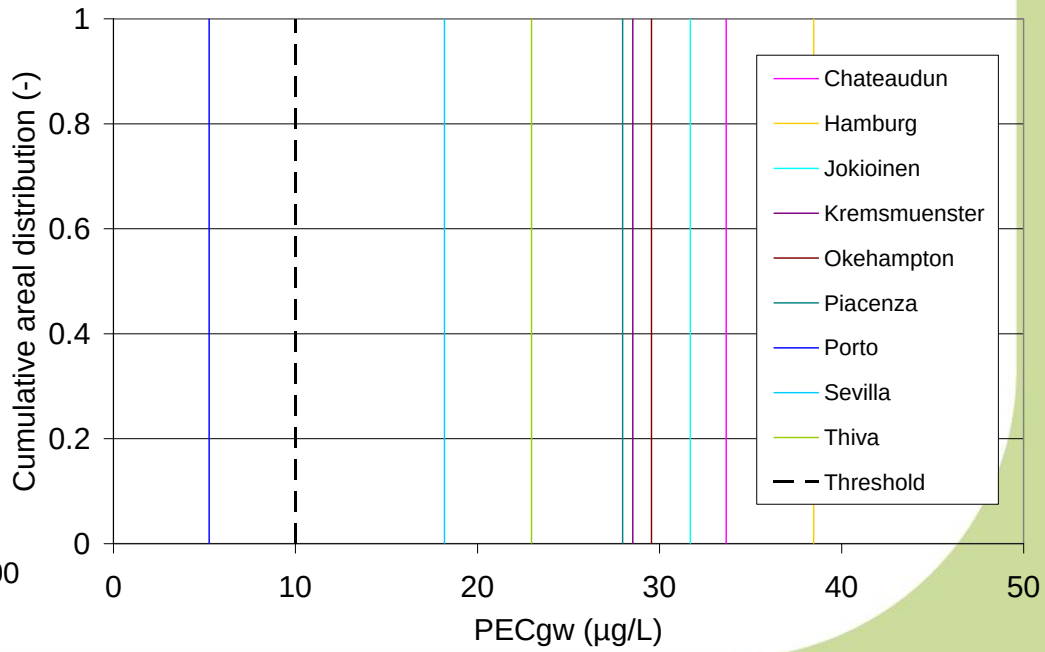
SubC in sugar beet

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

Parent



Non-relevant Metabolite

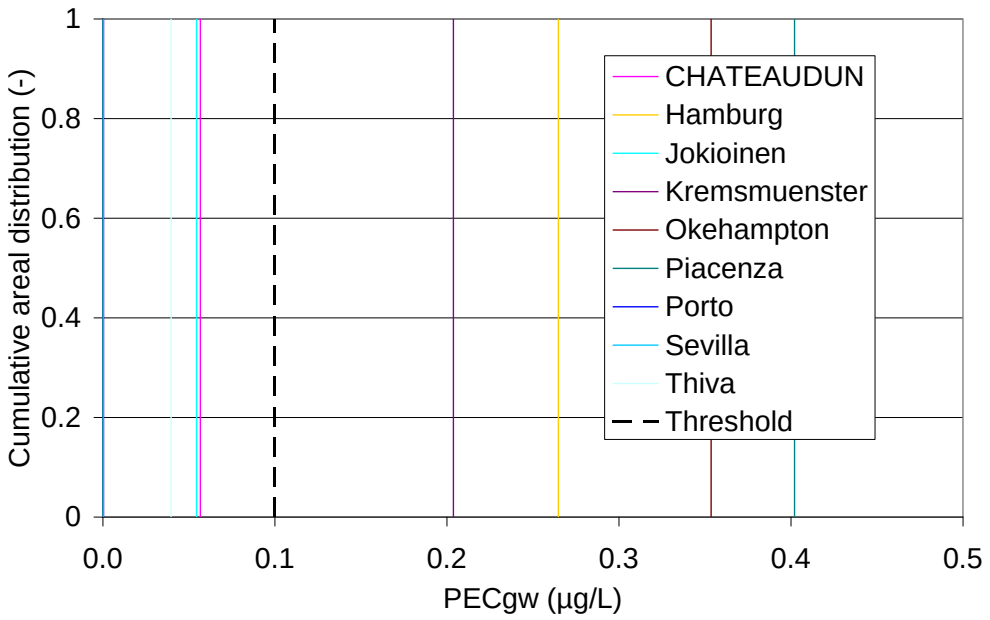


Mitigation: FOCUS Results

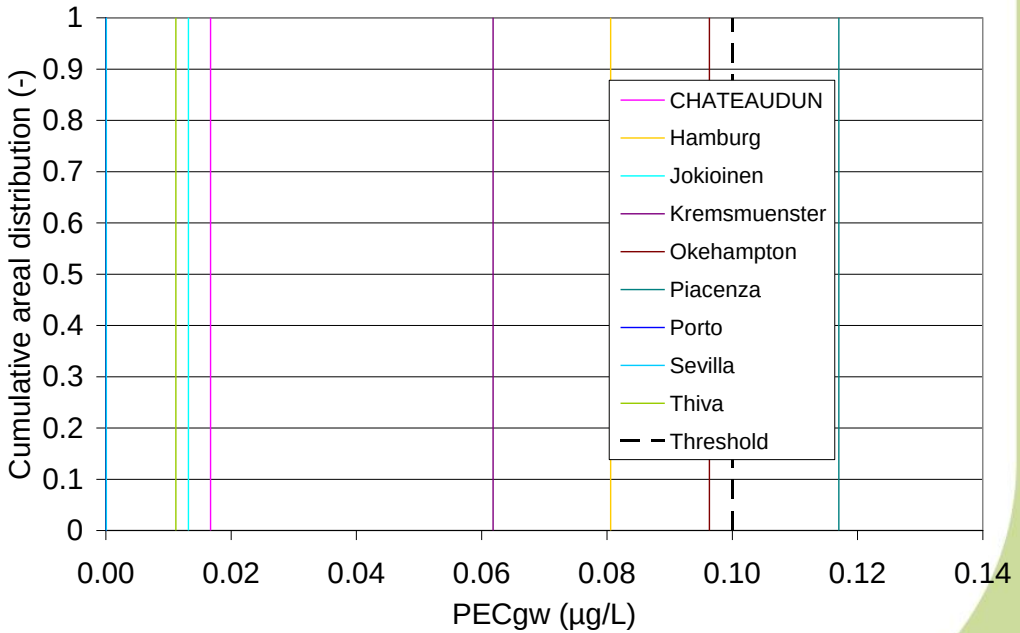
Test1 applied to winter wheat

➔ Parent and metabolite exceed threshold of 0.1 µg/L

Parent

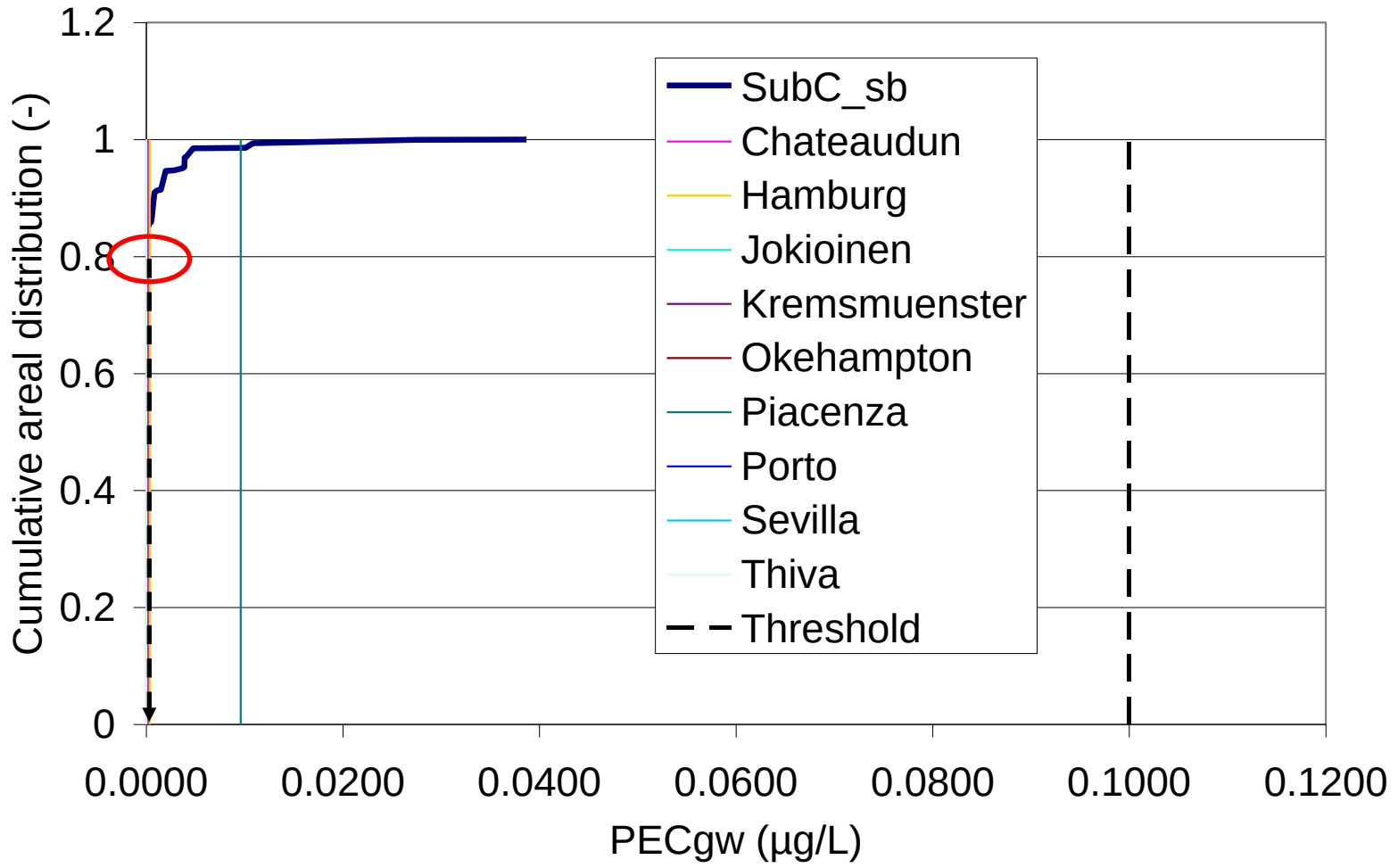


(relevant) Metabolite



Mitigation: FROGS Results

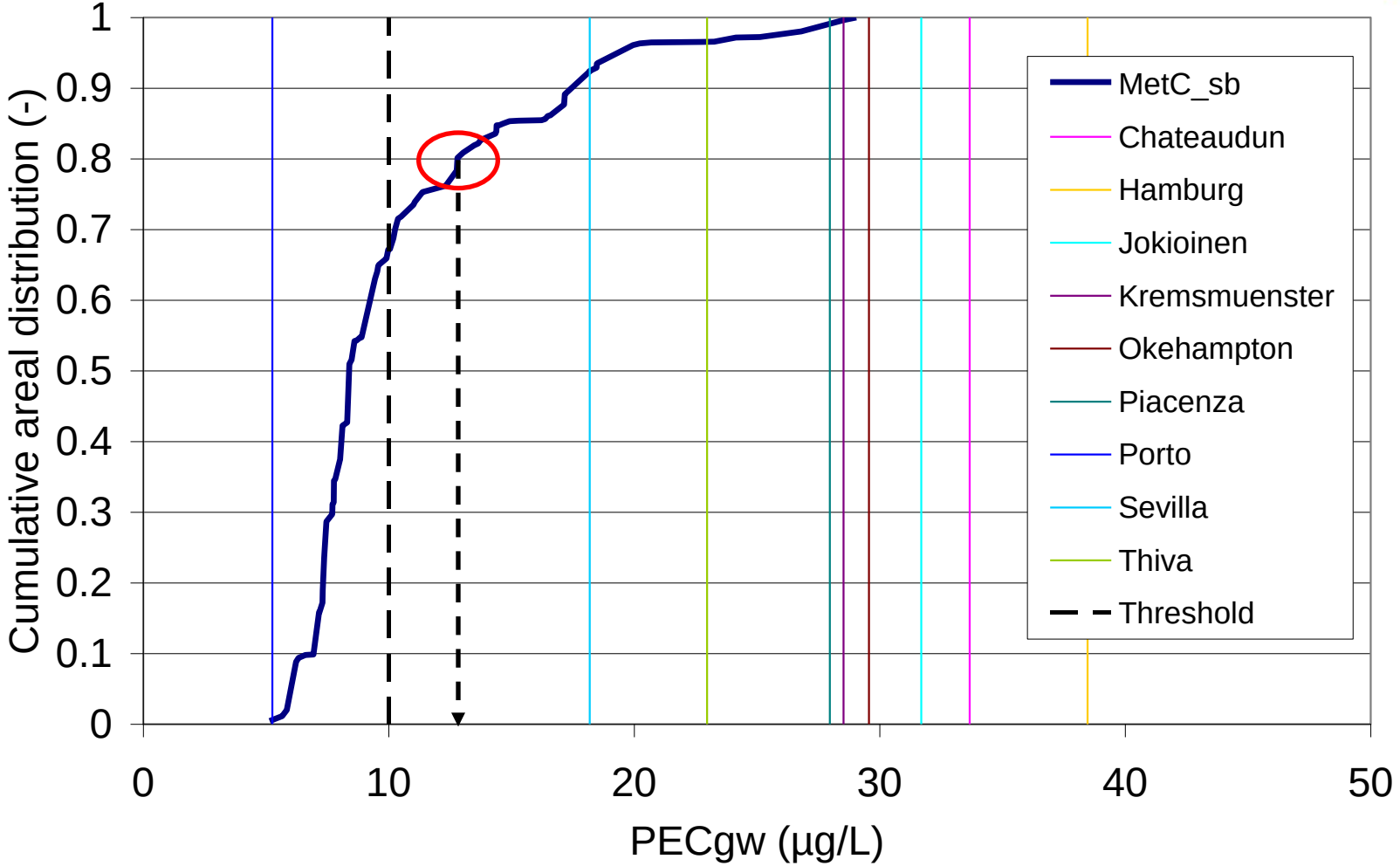
Parent SubC



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

Mitigation: FROGS Results

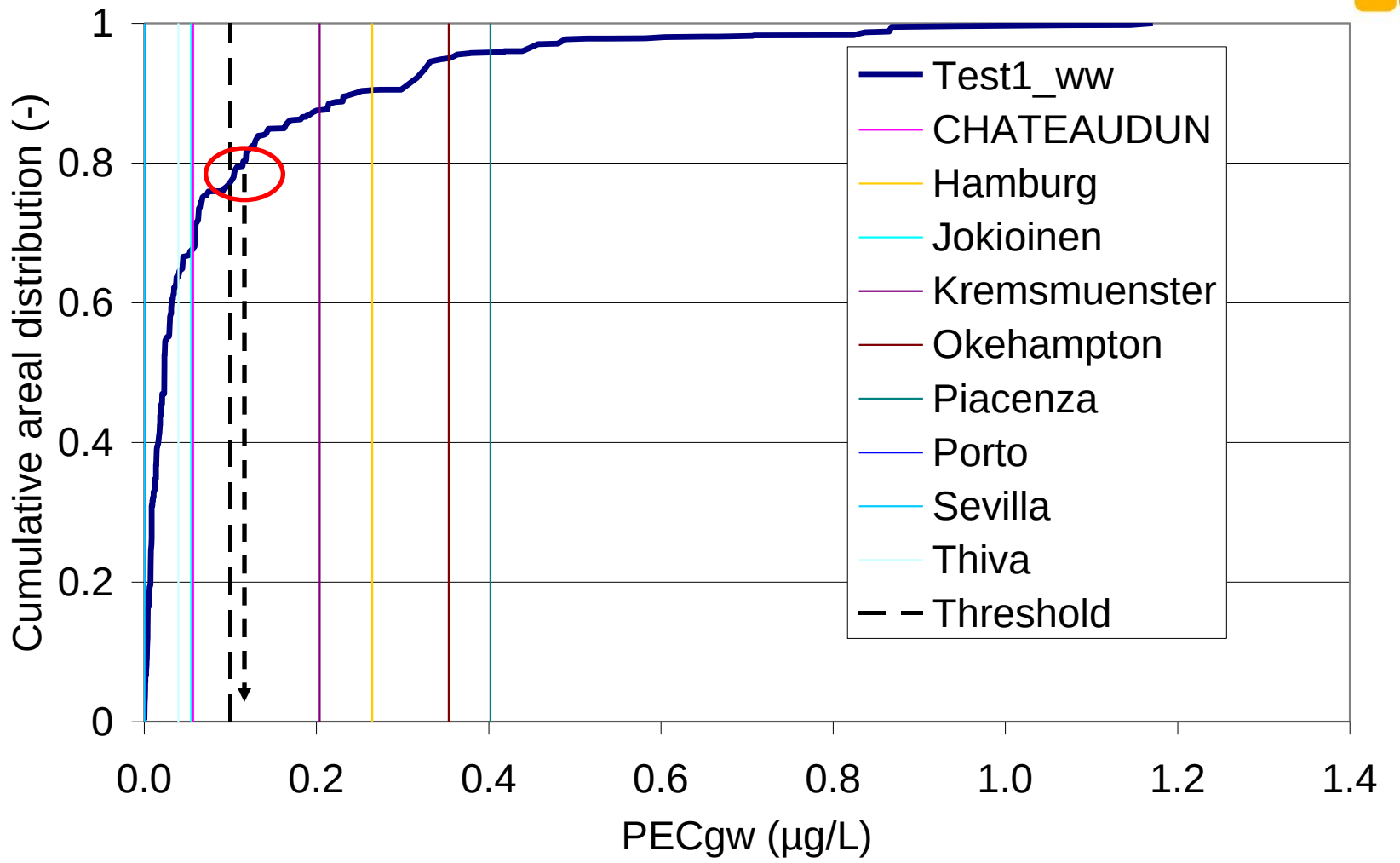
Metabolite MetC



80th spatial percentile of FROGS scenarios = 12.8 µg/L ➔ mitigation necessary

Mitigation: FROGS Results

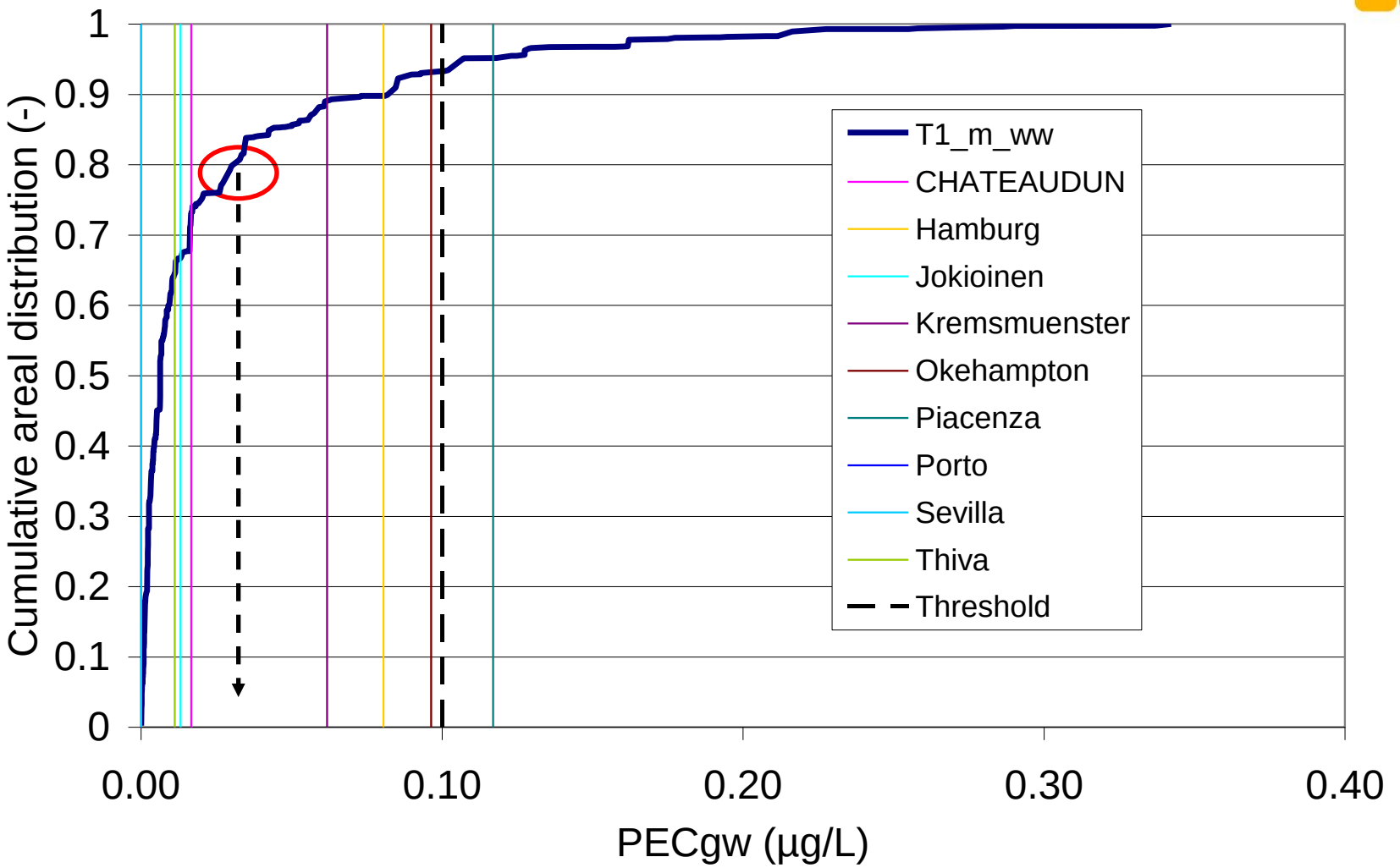
Parent Test1



80th spatial percentile of FROGS scenarios = 0.113 µg/L ➔ mitigation necessary

Mitigation: FROGS Results

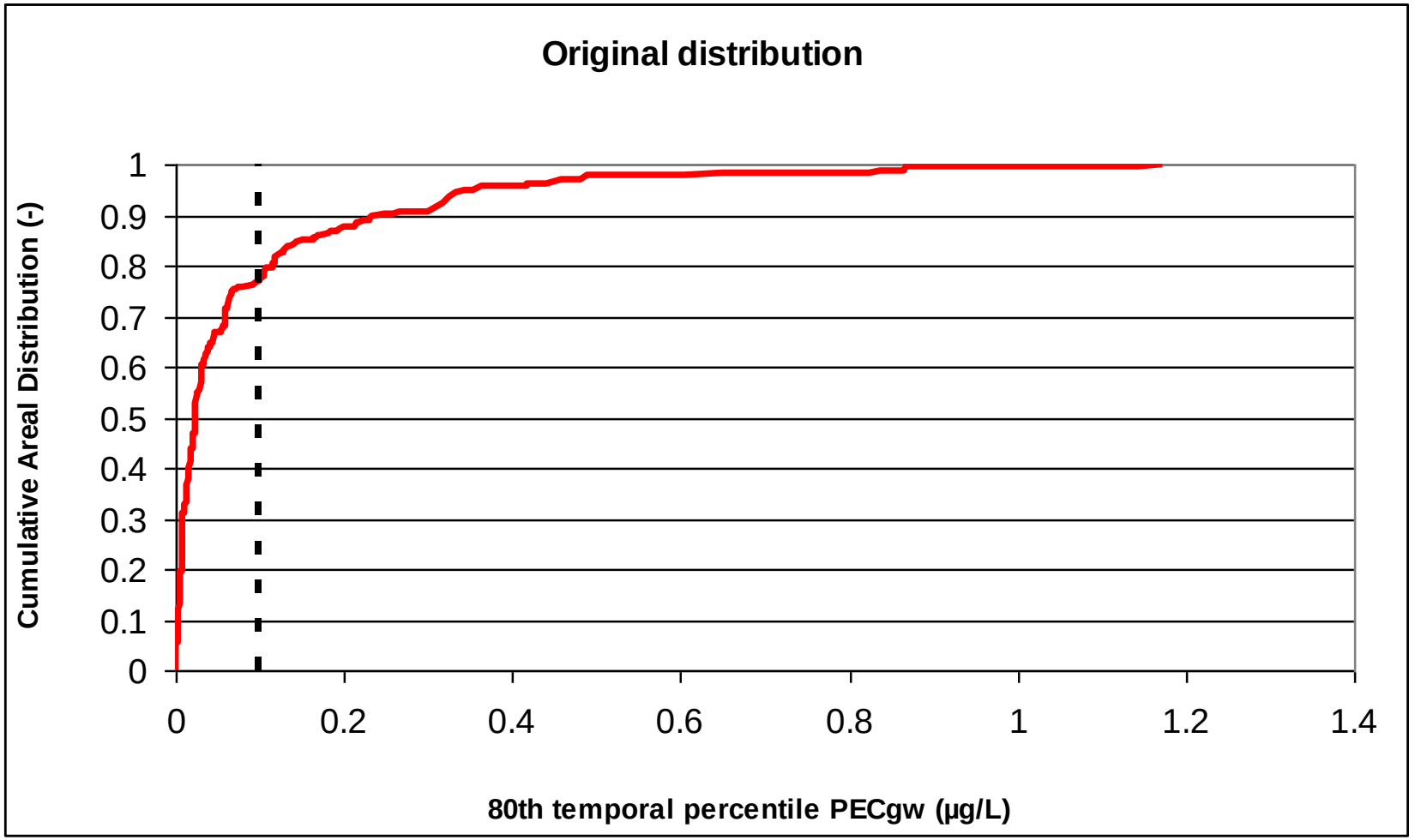
Metabolite Met1



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

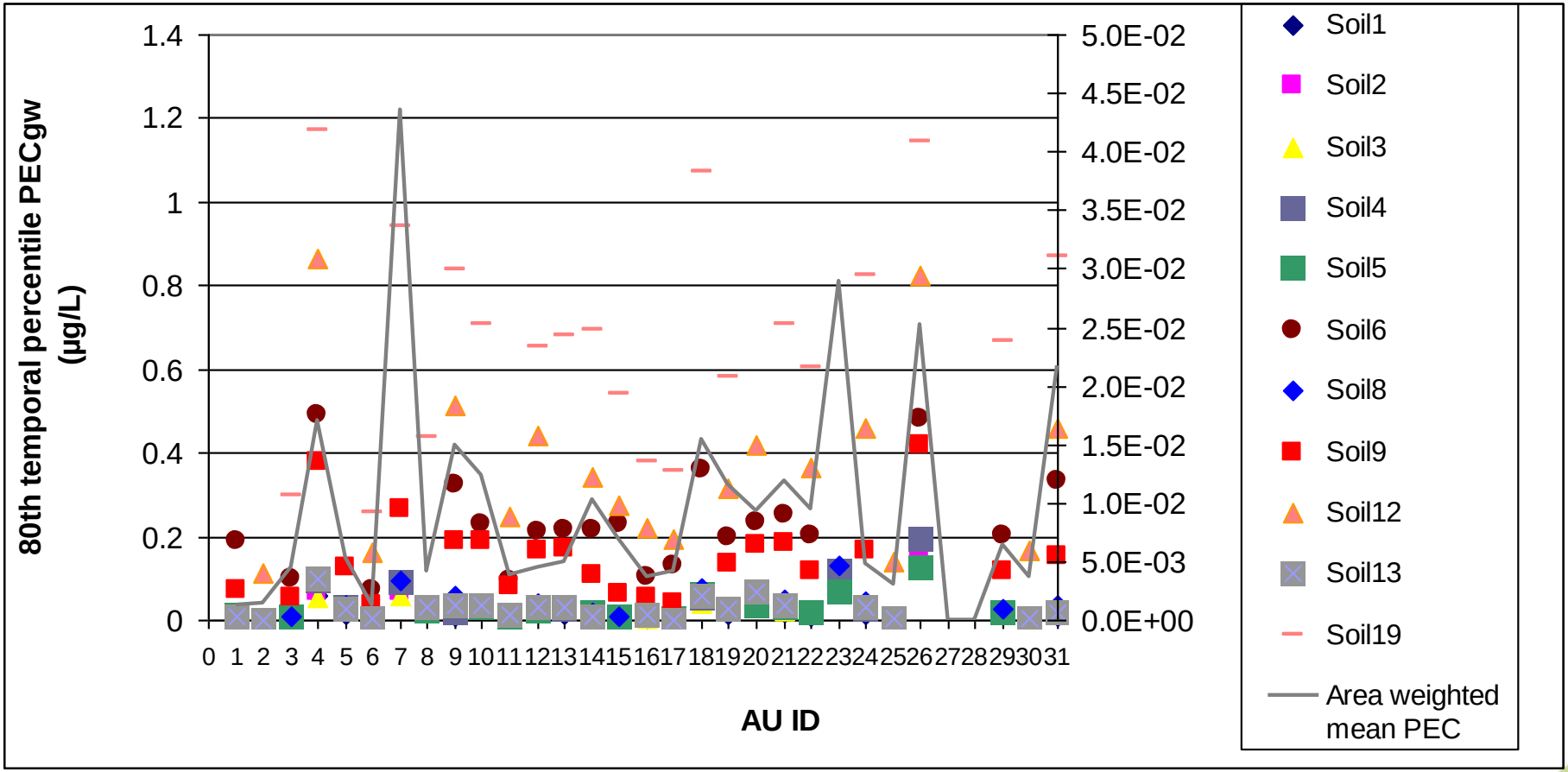
Mitigation: Example Substance Test1

Original Distribution (PEC = 0.113 µ/L)



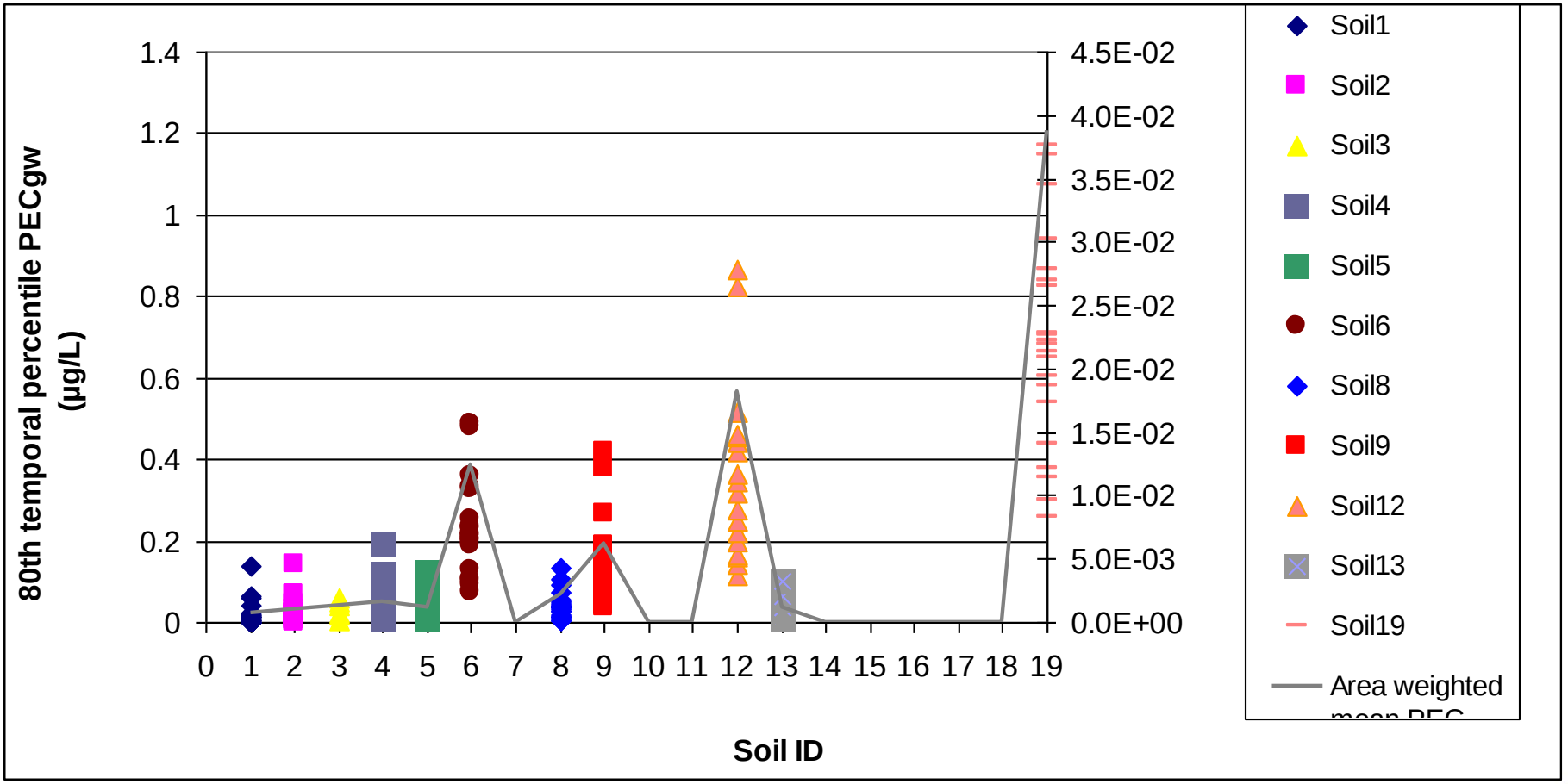
Mitigation: Example Substance Test1

PECs sorted by Agronomic United ➔ no clear pattern



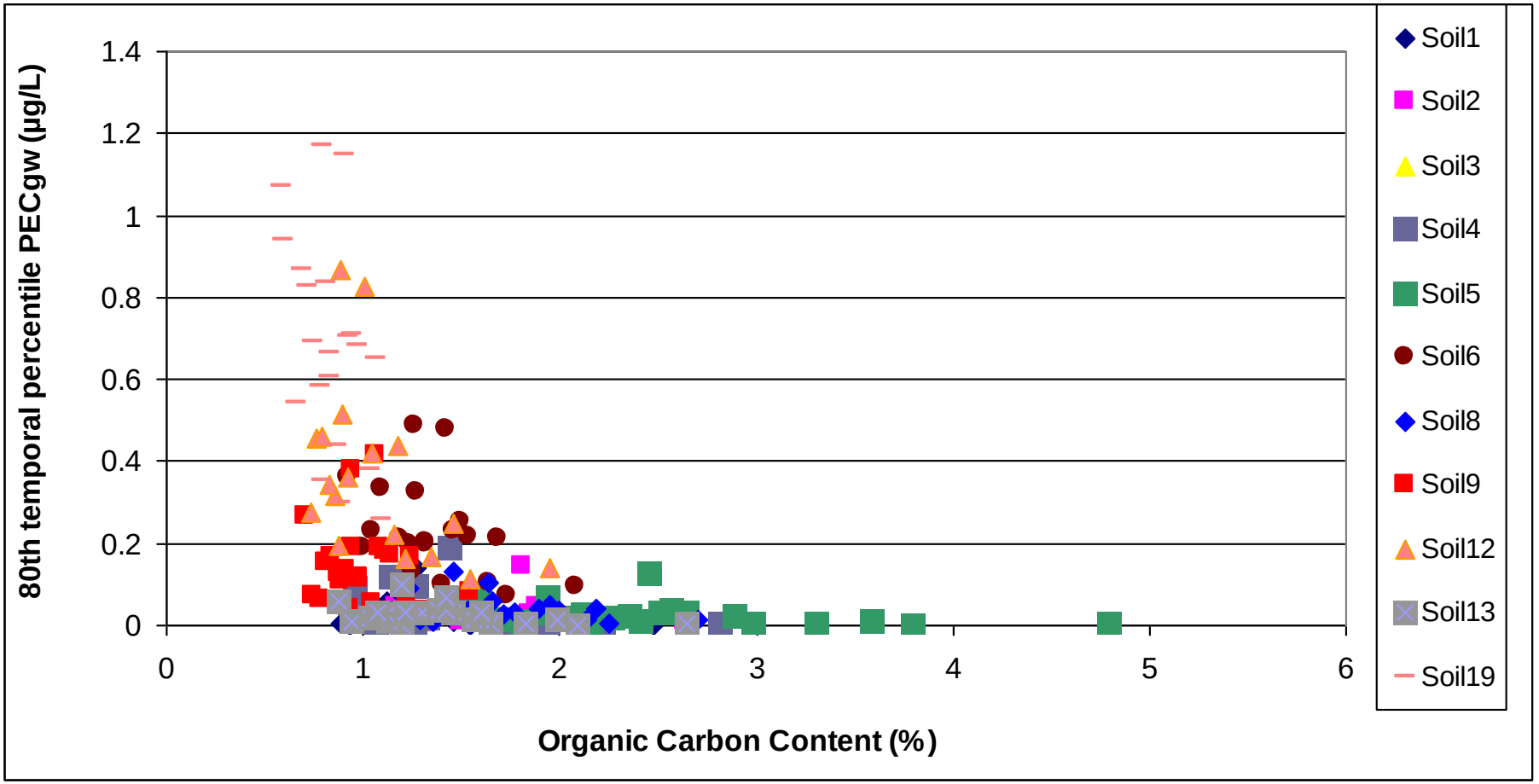
Mitigation: Example Substance Test1

PECs sorted by Soil ➔ PEC dependent on soil properties



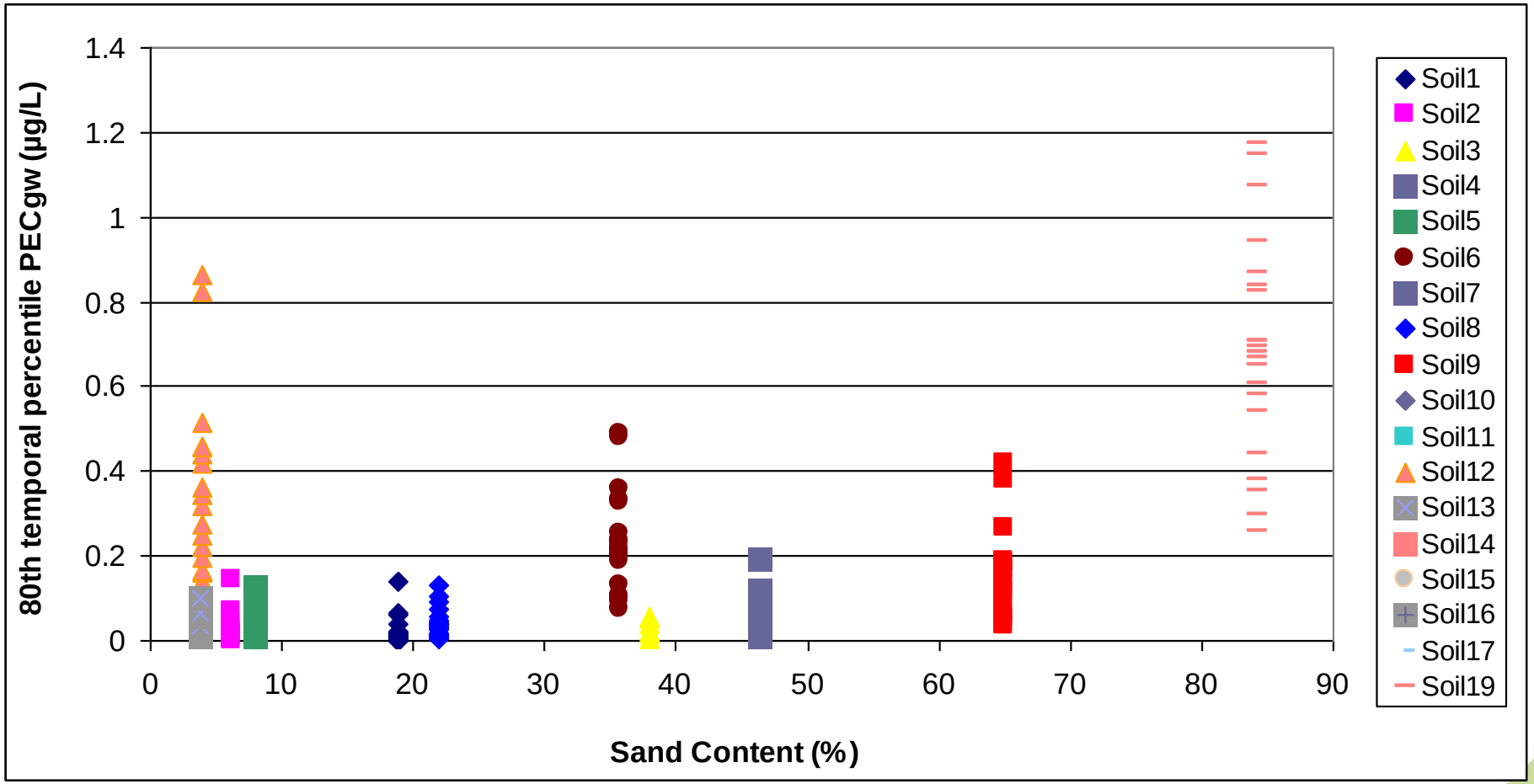
Mitigation: Example Substance Test1

PECs sorted by OC



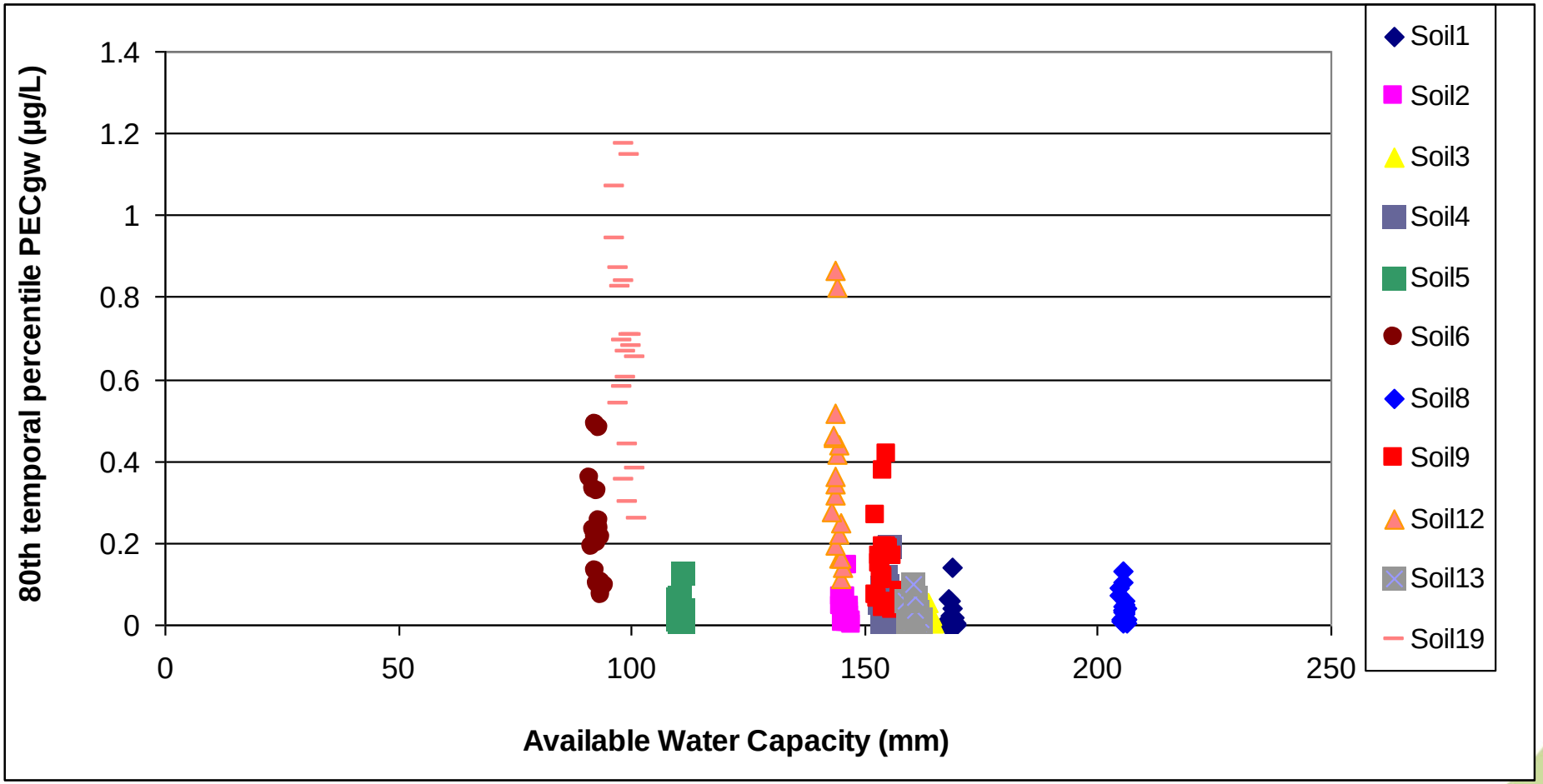
Mitigation: Example Substance Test1

PECs sorted by Sand content



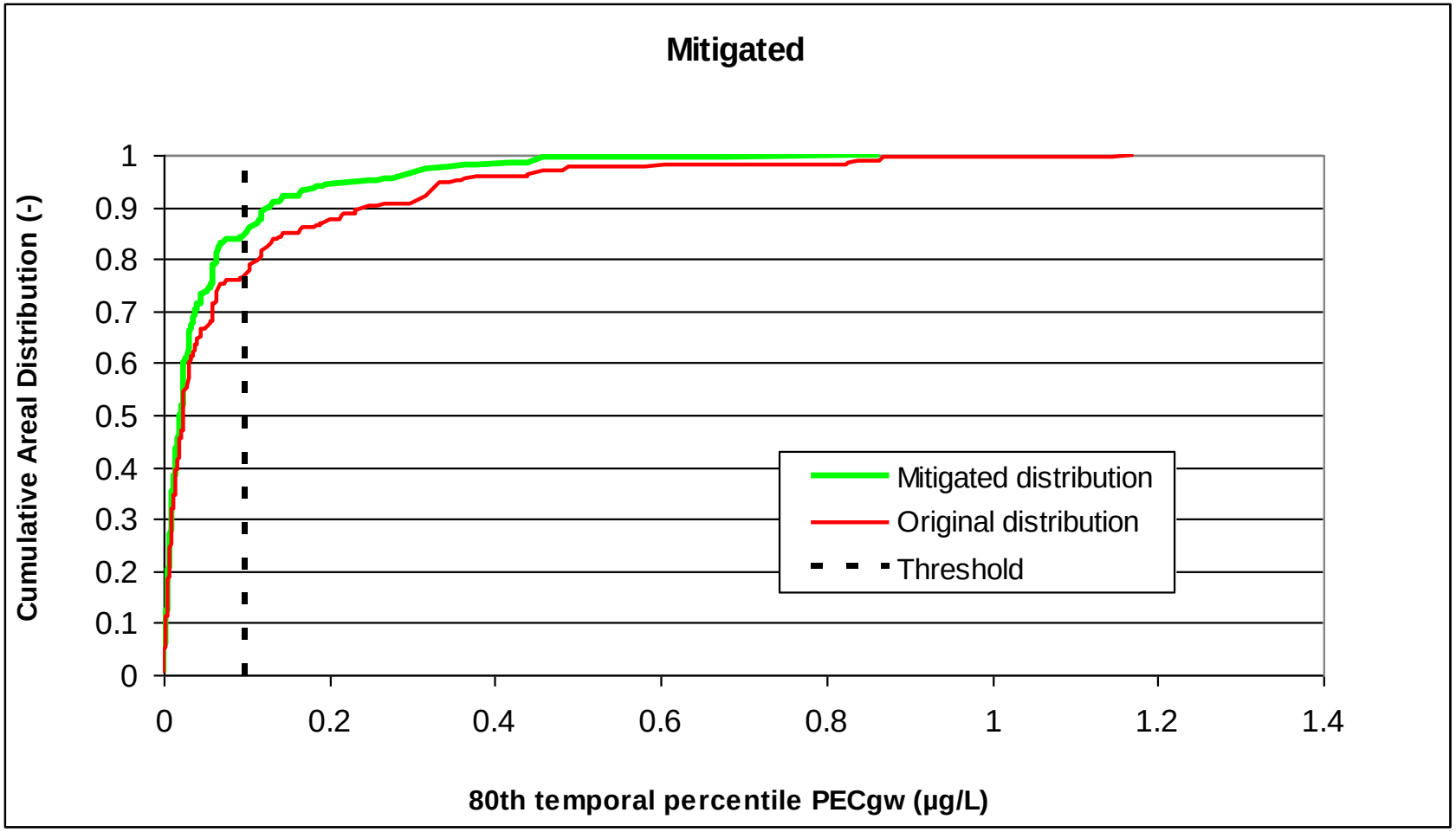
Mitigation: Example Substance Test1

PECs sorted by Available Water Capacity



Mitigation: Example Substance Test1

Mitigated by AWC (<100 mm)



PEC = 0.063 µg/L; Loss of area = 9.4%

Exercise 5: Mitigation

Exercise 5:

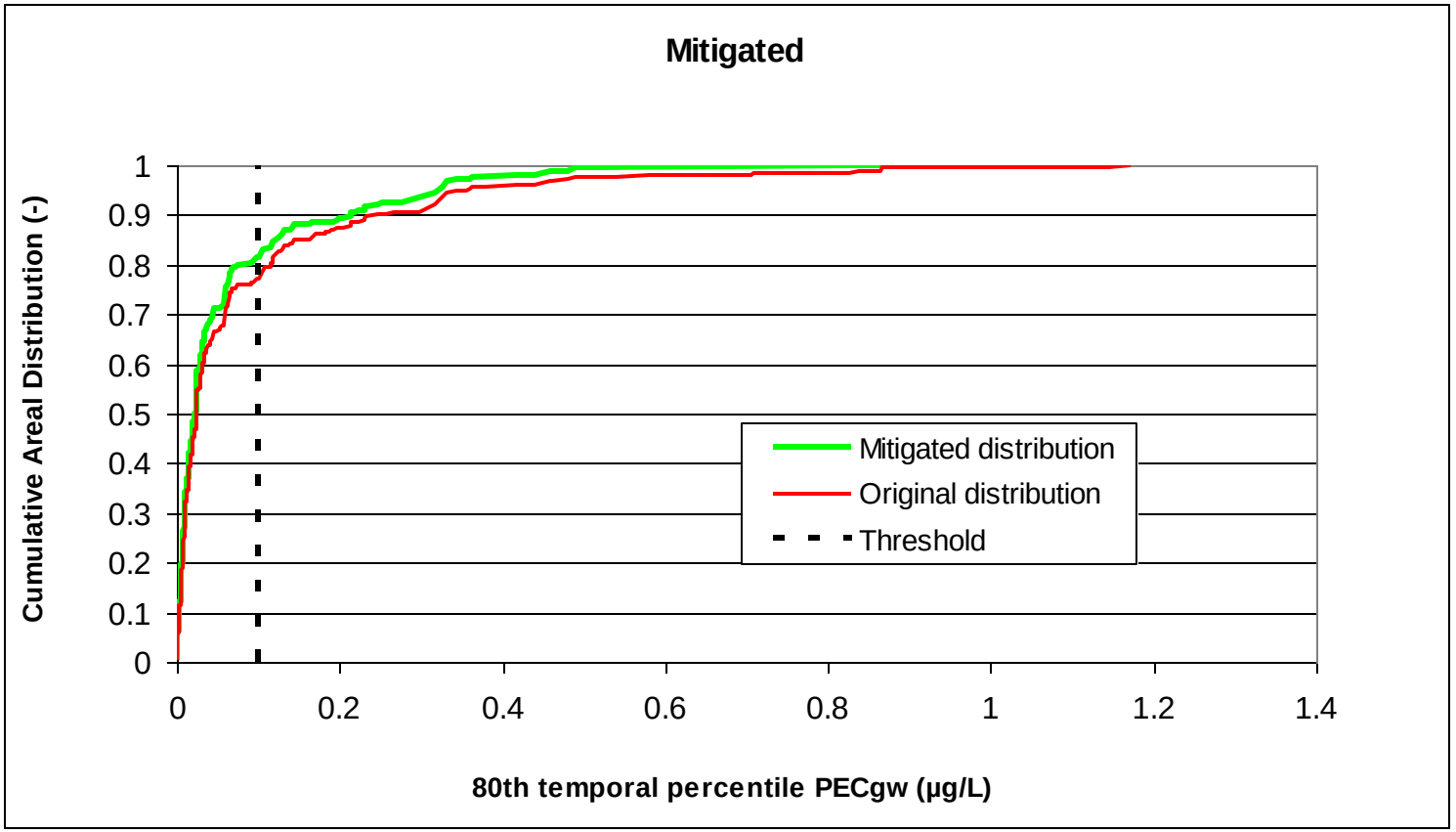
- Find complete „FROGS summary.txt“ files for both runs in folders „Exercise_SUBID_frogs_summary\FROGS summary.txt“. Import them each into a mitigation excel sheet.

- **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?

Exercise 5: Mitigation

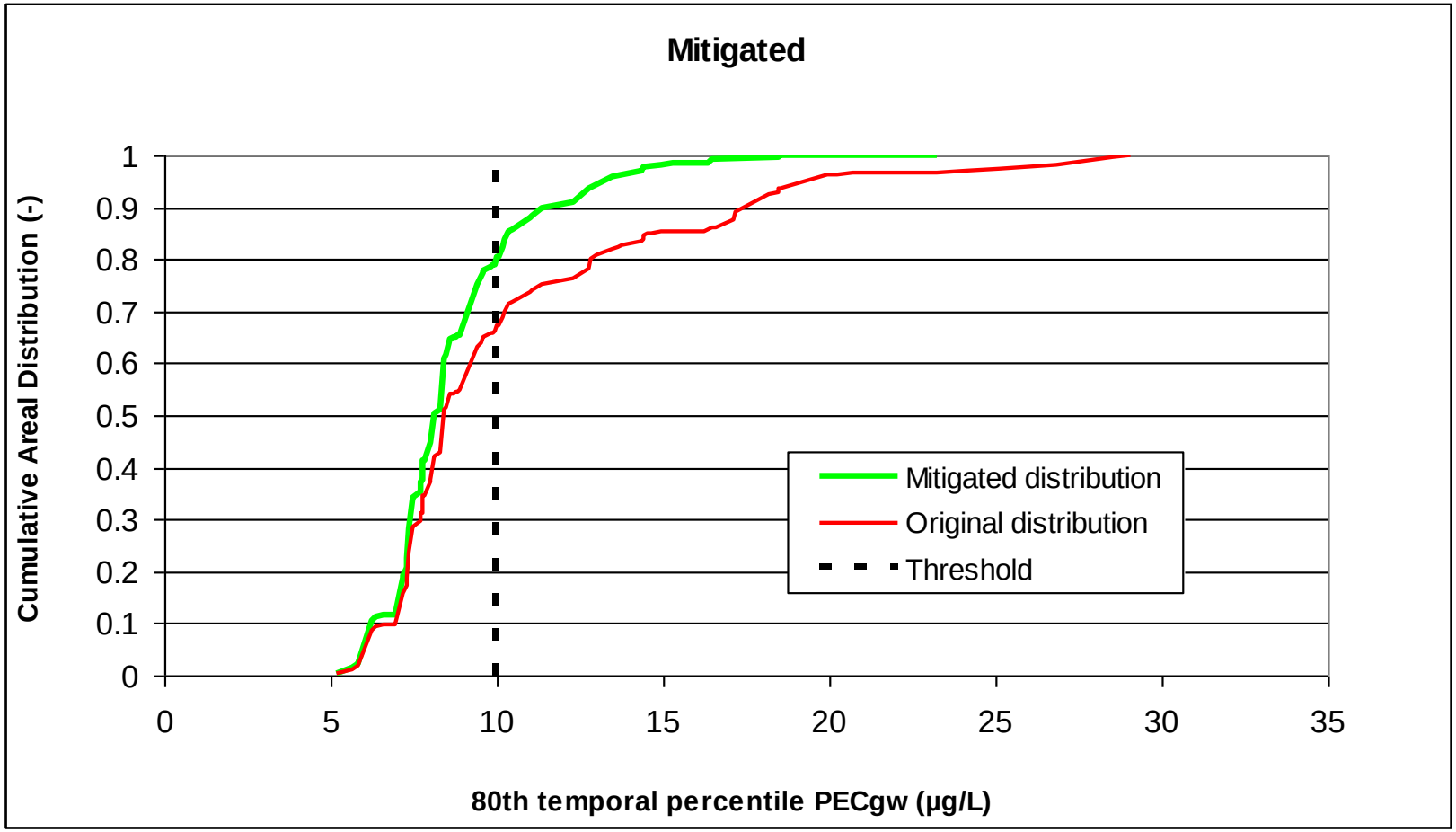
Test1: Mitigated by Sand content (< 60%)



PEC = 0.074 µg/L; Loss of area = 6.5%

Exercise 5: Mitigation

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