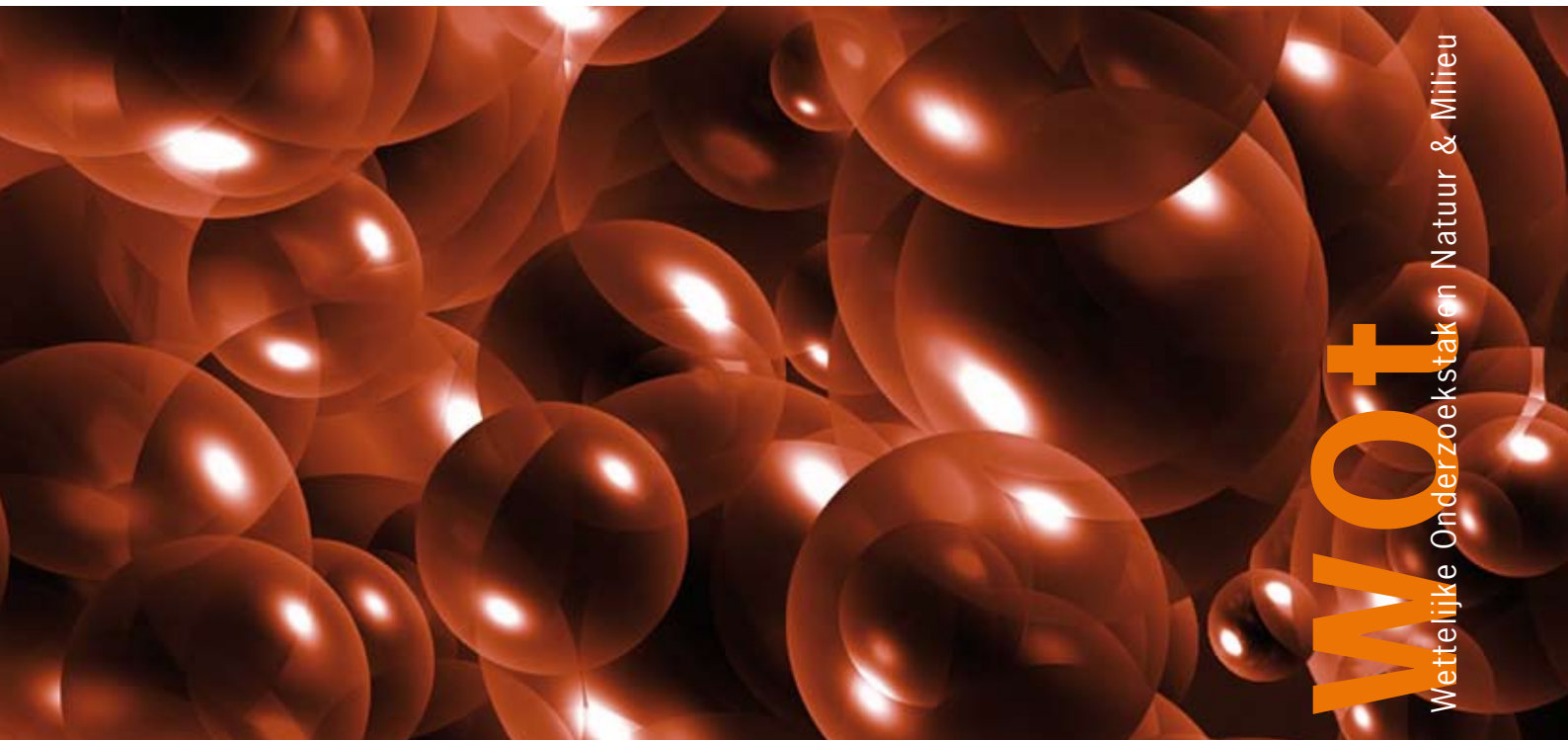


Documentation update for GeoPEARL_3.3.3

F. van den Berg
A. Tiktak
J.G. Groenwold
D.W.G. van Kraalingen
A.M.A. van der Linden
J.J.T.I. Boesten

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Wettelijke Onderzoekstaken Natuur & Milieu



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For quality of life

Documentation update for GeoPEARL_3.3.3

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Documentation update for GeoPEARL_3.3.3

F. van den Berg

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Werkdocument 103

Wettelijke Onderzoekstaken Natuur & Milieu

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Wageningen UR

Postbus 47, 6700 AA Wageningen

Tel: (0317) 48 07 00; fax: (0317) 41 90 00; e-mail: info.terra@wur.nl

Planbureau voor de Leefomgeving

Postbus 303, 3720 AH Bilthoven

Tel: (030) 274 27 45; fax: (030) 274 44 79; e-mail: info@pbl.nl

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Statutory Research Tasks Unit for Nature & the Environment, P.O. Box 47, NL-6700 AA Wageningen, The Netherlands
Phone: +31 317 48 54 71; Fax: +31 317 41 90 00; e-mail: info.wnm@wur.nl; internet: www.wotnatuurenmilieu.wur.nl

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Inhoud

1	New features in GeoPEARL_3.3.3	7
2	Bugs GeoPEARL_2.2.2 solved in GeoPEARL_3.3.3	8
3	Additions and Changes to User'guide of GeoPEARL_2.2.2	9
3.1	User's Guide of the GeoPEARL User Interface	9
3.1.1	Installation of the GeoPEARL User Interface	9
3.1.2	Getting started with the GeoPEARL User Interface	9
3.1.3	Viewing maps and graphs	13
3.2	User's Guide of the command-line version of GeoPEARL	15
3.2.1	Performing an assessment with the stand-alone version	15
3.2.2	File structure	15
3.2.3	Editing the control file	15
3.2.4	Example for the platform™ LSF system	15
	Literature	16
Appendix 1	Ploughing data file for crop-soil combinations in the Netherlands (plg file):	17
Appendix 2	The GeoPEARL_3.3.3 input file – Expert users	19

1 New features in GeoPEARL_3.3.3

The new GeoPEARL_3.3.3 contains an option to assess the persistence of compounds in the top layer of the soil at 2 or 7 years after the last application.

The new version also contains an option to select soils with a property within a range specified by the user. Only the soils for which the parameter values fall in the specified ranges are included in the assessment. The soil properties for which a range can be specified are:

- pH
- soil organic matter
- clay content
- silt content
- sand content
- sesqui-oxide content.

The new GeoPEARL version also considers ploughing practises in the cultivation of crops. For most crops, ploughing of the top 0.2 m of the soil occurs once a year. Moreover, the timing of the ploughing depends on soil category: sand, loam, clay or peat. Based on expert judgment, ploughing dates have been specified. The ploughing dates have been included in a separate schematization file, i.e. the .plg file. This file is shown in Appendix 1.

2 Bugs GeoPEARL_2.2.2 solved in GeoPEARL_3.3.3

The bugs that were found in GeoPEARL_2.2.2 have been solved in GeoPEARL_3.3.3. These were:

- For runs with a parent compound with a complex transformation scheme, sometimes duplicate output for a substance was generated. This error was due to duplicate entries in the table FraPrtDau. This bug has been eliminated by including a check on the substances in the transformation scheme (parent and metabolites) before writing the table FraPrtDau to the .cmp file of GeoPEARL.
- Runs for a compound with more than 4 metabolites gave an error message. This has been solved by increasing the maximum number of compounds in a single assessment from 5 to 20.

Compatibility

GeoPEARL_3.3.3 is fully compatible with GeoPEARL_2.2.2. There will be no loss of data in your database created by GeoPEARL_2.2.2, as GeoPEARL_3.3.3 will upgrade your database automatically when you open it for the first time with GeoPEARL_3.3.3.

GeoPEARL_3.3.3 can be used on VISTA platforms.

3 Additions and Changes to User'guide of GeoPEARL_2.2.2

This section describes the changes and the additions for the update of the GeoPEARL_2.2.2 user manual (Tiktak *et al.*, 2006) to be used in combination with GeoPEARL_3.3.3.

3.1 User's Guide of the GeoPEARL User Interface

See report GeoPEARL_2.2.2 – Chapter 2

3.1.1 Installation of the GeoPEARL User Interface

See report GeoPEARL_2.2.2 – Section 2.2

- Before using GeoPEARL, you have to install the model. The model comes in a self-extracting archive, called `geoppearl_3_3_3.exe`. This archive is available at the download page of the PEARL website, which is at the address <http://www.geoppearl.pesticidemodels.eu>.
- Figure 3, first step: Download `geoppearl_3_3_3.exe` from the address <http://www.geoppearl.pesticidemodels.eu>.

3.1.2 Getting started with the GeoPEARL User Interface

See report GeoPEARL_2.2.2 – Section 2.3

In GeoPEARL_3.3.3 two additional features have been added. These features can be used in the step 'Select plots and/or persistency option', which is introduced after the step to generate assessments as described in section 2.3 of the User's guide of GeoPEARL_2.2.2.

The additional features are:

- Select plots on the basis of a range of values for the soil property selected by the user;
- Select the option to obtain output on pore water concentrations and concentrations in soil at predefined endpoints after the last application.

The steps in a GeoPEARL assessment including the new features are shown in Figure 1.

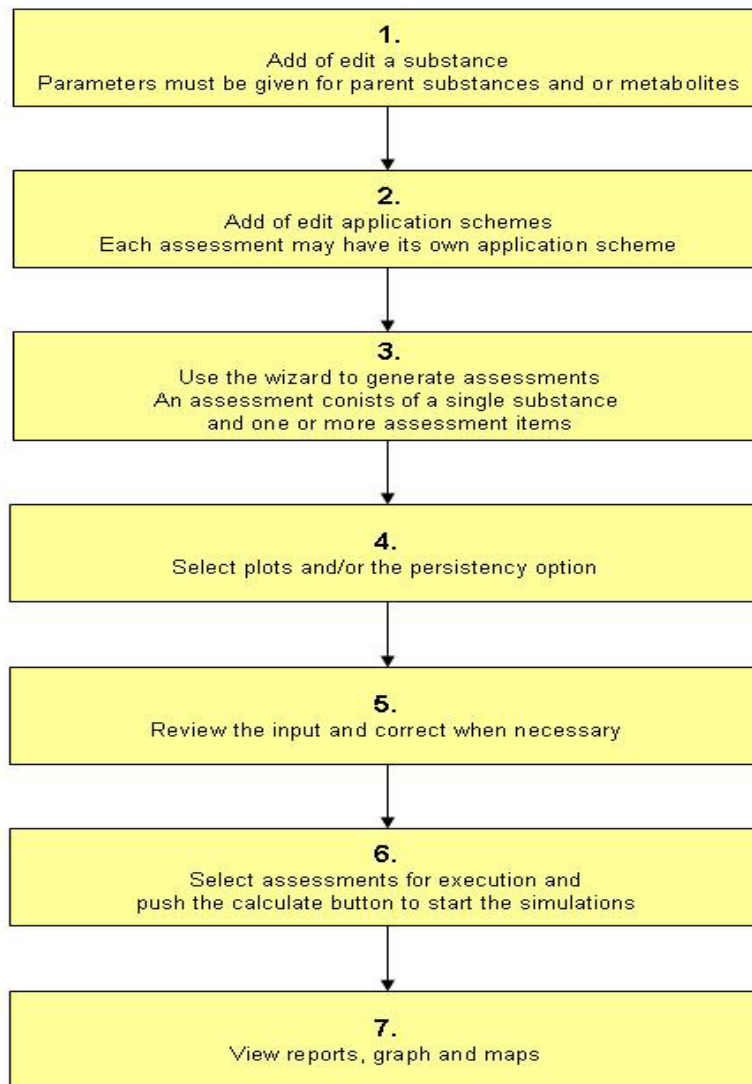


Figure 1. Major steps of a GeoPEARL assessment including the new option to select plots and the option to assess the persistency of the substance in the soil.

Figure 5 in the manual GeoPEARL_2.2.2 is replaced by Figure 2. The new main screen includes the option to select soils (the 'Plot selection' button) as well as the option to obtain additional output on pore water concentrations and soil contents at predefined endpoints as required for the persistency assessment according to the new Dutch decision scheme (the checkbox 'Persistence output'). On top of the screen a new button 'Plots Info' has been added to view the results of the selection of a range of values for a soil property on the number of available plots.

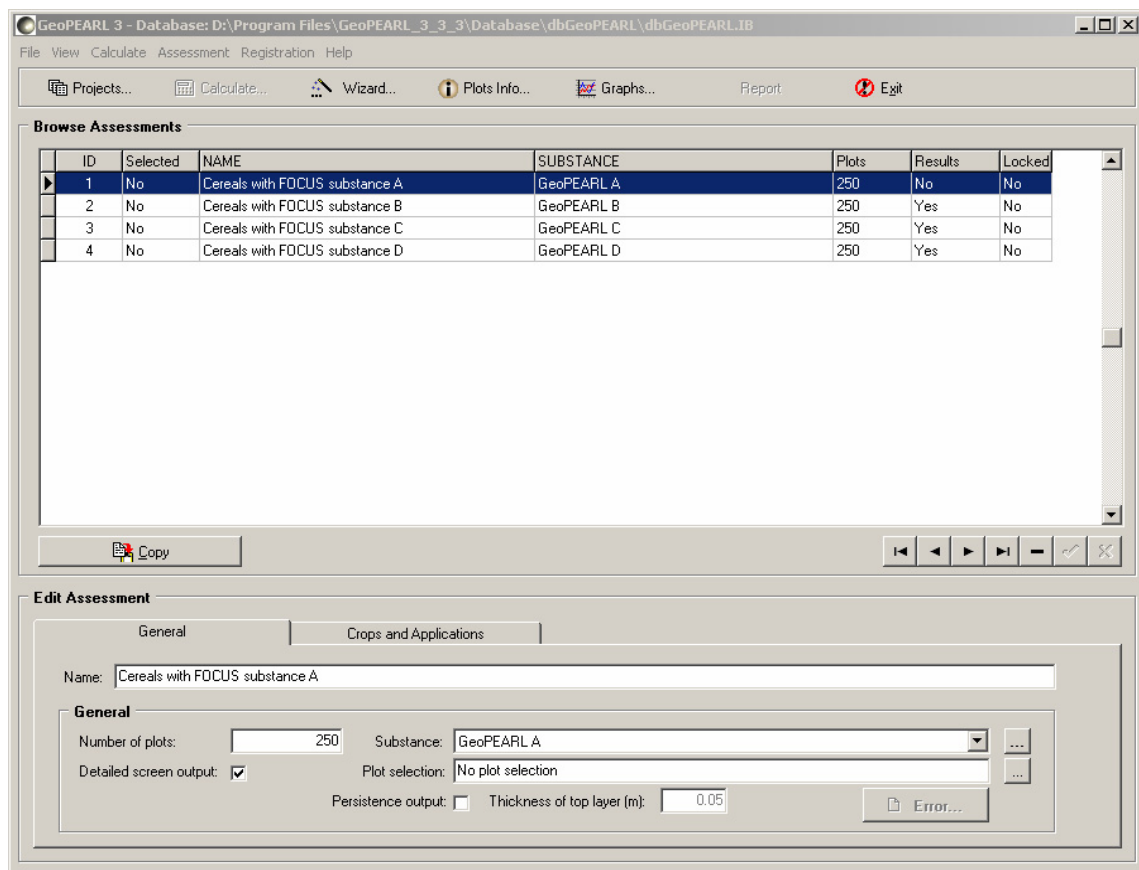


Figure 2. The main form of the GeoPEARL_3_3_3 User Interface.

After clicking on the 'Plot selection' button, the soil property of interest can be selected and the user has to specify the range of values for this property (See Figure 3). The soil properties that can be selected are::

- pH
- Organic matter
- Clay fraction
- Silt fraction
- Sand fraction
- Sesqui-oxide

After selection of a property and specification of the range, click on 'Close'. Next a message appears on the screen showing the number of plots in the selection.

The results of the plot selection are also shown after clicking on the button 'Plots Info'. An example of the report on the plot selection is shown in Figure 4. Only those plots are included in the selection that are relevant for the crop(s) included in the assessment. If the number of plots remaining for the assessment is insufficient then the user has to adjust the range of values for the soil property.

GeoPEARL 3 - Plot selection

No

pH dependent Lower bound: [2.7] Upper bound: [7.8] (data between 2.7 and 7.8, unit = -)

Organic matter content dependent Lower bound: [0.001] Upper bound: [0.95] (data between 0.001 and 0.95, unit = kg.kg-1)

Clay fraction dependent Lower bound: [0.002] Upper bound: [0.71] (data between 0.002 and 0.71, unit = kg.kg-1 mineral parts)

Silt fraction dependent Lower bound: [0] Upper bound: [0.91] (data between 0 and 0.91, unit = kg.kg-1 mineral parts)

Sand fraction dependent Lower bound: [0.007] Upper bound: [0.998] (data between 0.007 and 0.998, unit = kg.kg-1 mineral parts)

Sesquioxides content dependent Lower bound: [9] Upper bound: [1192] (data between 9 and 1192, unit = mmol.kg-1)

[Close] [Cancel]

Figure 3. The plot selection form.

GeoPEARL 3.3.3 Plots Info: "Assessment14"

Date: 02/07/2007

"pH dependent" plot selection was chosen with:
 lower limit : 5.5000
 upper limit : 6.6000
 selected plots : 1272

Plots selected : 1272

Crop name	Number of plots for crop
Potatoes	1043
Legumes	920
Fallow	1256
Cereals	1089
LeafVegetables	771
Floriculture	1009

Figure 4. The report on the number of selected plots for the crops in the assessment using the 'Plots Info' button.

The persistency option can be selected by clicking on the check box on the right-hand side of 'Persistency output'. Next the user has to specify the thickness of the top layer for which the pesticide content and pore water concentration is calculated. After completion of the assessment, a section with the persistency output is included in the GeoPEARL report. An example of the information added is shown in Figure 5.

GeoPEARL_3.3.3 REPORT: "Assessment 10"

Summary for persistence

For the assessment of persistence in the Dutch pesticide registration procedure the following quantities are reported below:

- average total content of substance in the top layer used for evaluation of persistence
- average pore water concentration of substance in the top layer used for evaluation of persistence.

The report below describes these two quantities for different time windows for averaging as indicated and for three moments in time that are linked to two protection goals as follows:

- the quantity as calculated 2 years after the last application of the pesticide, linked to the Community Recovery Principle (called 'CRP')
- the quantity as calculated 7 years after the last application of the pesticide, linked to the Ecological Threshold Principle (called 'ETP')

See for background of the protection goals:

Linden AMA van der, JJTI Boesten, TCM Brock, GMA van Eekelen, FMW de Jong, M Leistra, MHMM Montforts & JW Pol, 2006. Persistence of plant protection products in soil; a proposal for risk assessment. RIVM Report 601506008/2006, Bilthoven, Netherlands, 105 pp. available at:

<http://www.rivm.nl/bibliotheek/rapporten/601506008.html>

Persistence output was based on a thickness layer of 0.05 meter

Overall persistence results:

Time weighted average content (mg/kg) in top layer

Time window	CRP (mg/kg)	ETP (mg/kg)
0 days	7.7035934	6.5161340
7 days	7.7013944	6.5139219
14 days	7.6986284	6.5108949
21 days	7.6957843	6.5078690
28 days	7.6928763	6.5050522
56 days	7.6797412	6.4932554
180 days	7.6159809	6.4354921
365 days	7.5523712	6.3750764

Time weighted average pore water concentration (ug/L) in top layer

Time window	CRP (ug/L)	ETP (ug/L)
0 days	0.0008109	0.0006729
7 days	0.0008088	0.0006708
14 days	0.0008088	0.0006708
21 days	0.0008099	0.0006719
28 days	0.0008078	0.0006698
56 days	0.0008068	0.0006688
180 days	0.0007988	0.0006618
365 days	0.0007913	0.0006553

Figure 5: The output on the persistency of the substance at the predefined end points as included in the GeoPEARL report.

3.1.3 Viewing maps and graphs

See report GeoPEARL_2.2.2 – Section 2.12.2

After running the assessment, additional graphs can be shown using the persistency output. These new graphs are related to the 'Area of Use' as well as to the 'Area of Crop' (Figs. 6 and 7).

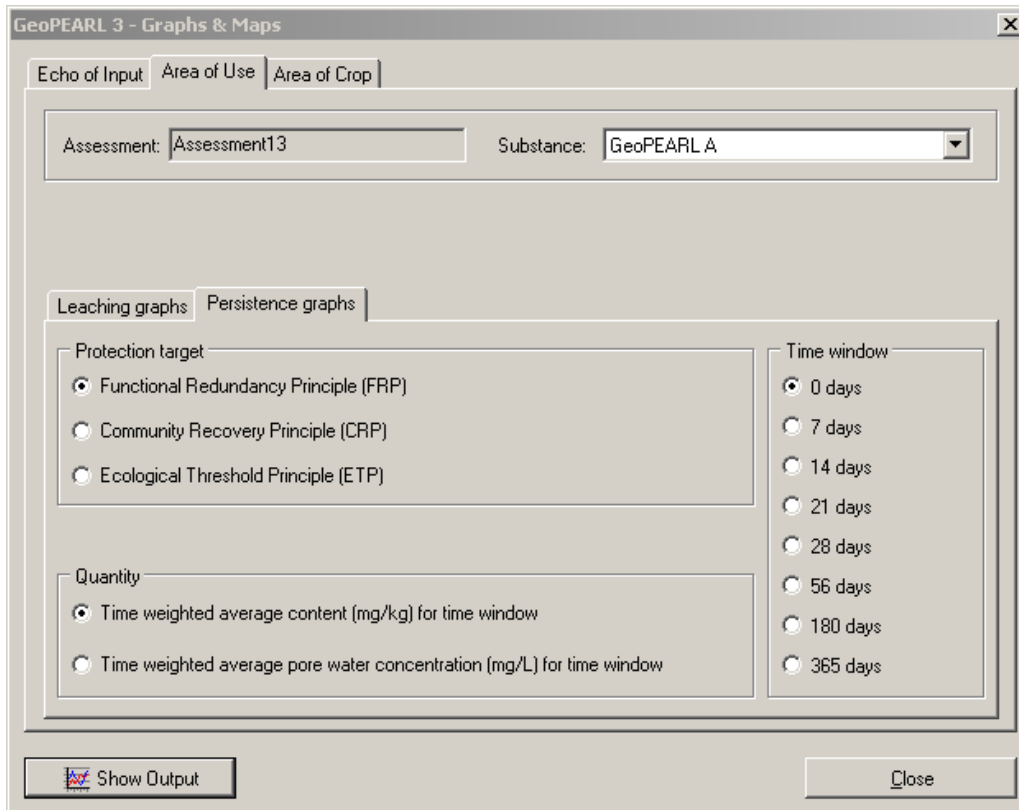


Figure 6. The new persistence graphs for the area of use.

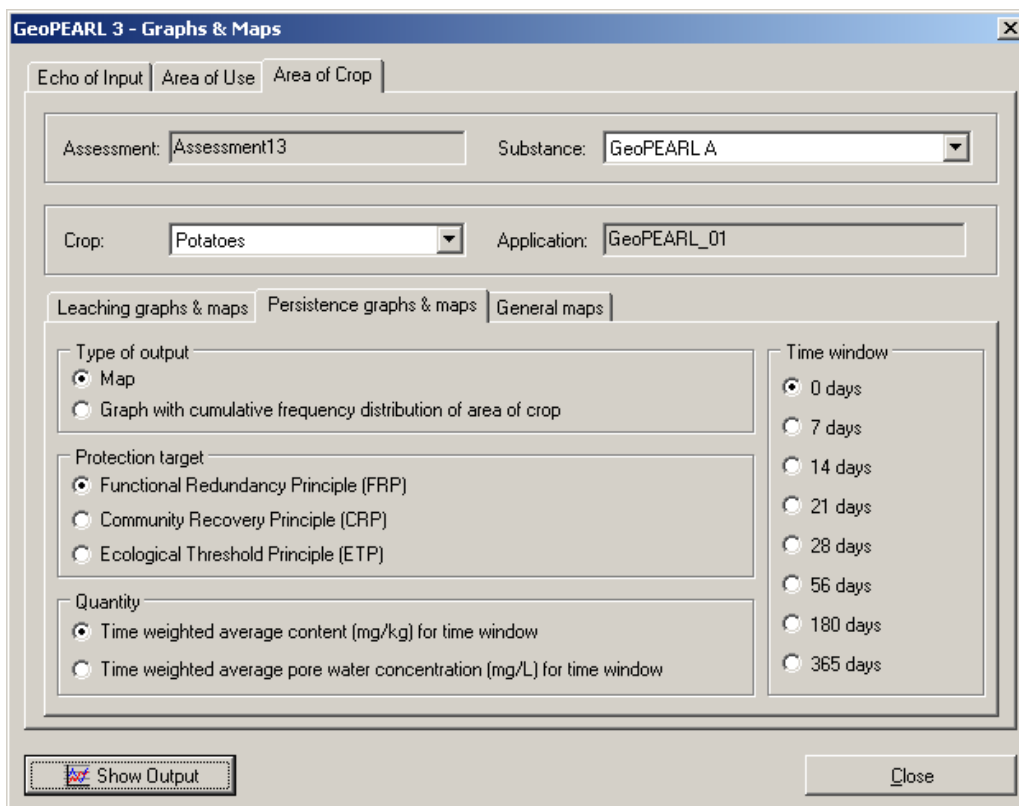


Figure 7. The new persistence graphs for the area of crop

3.2 User's Guide of the command-line version of GeoPEARL

See report GeoPEARL_2.2.2 – Chapter 3

3.2.1 Performing an assessment with the stand-alone version

See report GeoPEARL_2.2.2 – Section 3.1

Download the 'geoppearl_3_3_3_ascii.exe' self-extracting archive from the PEARL website to get the input files for the stand-alone version of GeoPEARL. Put the files preferably into a directory *without spaces*.

3.2.2 File structure

See report GeoPEARL_2.2.2 – Section 3.2

GeoPEARL generates an input file, i.e. 'PlotsIncludes.inc', listing the included plots for the assessment.

3.2.3 Editing the control file

See report GeoPEARL_2.2.2 – Section 3.6

An example of the new .geo file is presented in Appendix 2.

3.2.4 Example for the platform™ LSF system

See report GeoPEARL_2.2.2 – Section 3.11.1

Reference to 'GeoPEARL_2_2_2' should be replaced by 'GeoPEARL_3_3_3'

Literature

Tiktak, A., Van der Linden, A.M.A., Boesten, J.J.T.I., Kruijine, R., Kraalingen, D. and F. van den Berg, 2006. The GeoPEARL model, version_2.2.2. Part II: User guide and model description update. RIVM report 716601008/2004-2006

Appendix 1 Ploughing data file for crop-soil combinations in the Netherlands (plg file):

```

*-----
*
*       File containing           the ploughing parameters for the Netherlands.
*
*-----

* table CTB_Crops
* 1 Potatoes
* 2 Strawberries
* 3 Asparagus
* 4 SugarBeets
* 5 LeafVegetables
* 6 plants_for_commercial_purposes
* 7 Floriculture
* 8 FlowerBulbs
* 9 TreeNursery
* 10 Fallow
* 11 FruitCulture
* 12 Cereals
* 13 Grass
* 14 GrassSeed
* 15 GreenManuring
* 16 Vegetables
* 17 Cannabis
* 18 Silviculture
* 19 Cabbage
* 20 Maize
* 21 RemainingAgriculturalCrops
* 22 Legumes
* 23 Leek
* 24 Onions
* 25 TotalAgriculturalArea

* 26 TotalNonUrbanArea
* end_table

*-----
* Column 1: Crop Number
* Column 2: Ploughing date for culture on sandy soil (dd-mm)
* Column 3: Ploughing date for culture on clayey soil (dd-mm)
* Column 4: Ploughing date for culture on loamy soil (dd-mm)
* Column 5: Ploughing date for culture on peaty soil (dd-mm)

table PloughingData
1      15-Mar  15-Nov  15-Feb  None
2      31-Jul  15-Nov  15-Feb  None
3      01-Mar  15-Dec  15-Feb  None
4      31-Mar  15-Nov  15-Feb  None
5      31-Mar  15-Nov  15-Feb  None
6      28-Feb  15-Nov  15-Feb  None
7      31-Mar  15-Nov  15-Feb  None
8      15-Oct  15-Dec  15-Feb  None
9      None   None   None   None
10     None   None   None   None
11     None   None   None   None
12     15-Oct  15-Nov  15-Feb  None
13     31-Aug  None   None   None
14     31-Aug  None   None   None
15     15-Oct  15-Dec  15-Feb  None
16     31-Mar  15-Dec  15-Feb  None
17     15-Oct  15-Nov  15-Feb  None
18     None   None   None   None
19     31-Mar  15-Nov  15-Feb  None

```

20	15-Apr	15-Nov	15-Feb	None
21	31-Mar	15-Nov	15-Feb	None
22	01-Mar	15-Dec	15-Feb	None
23	15-Aug	15-Nov	15-Feb	None
24	31-Mar	15-Nov	15-Feb	None
25	31-Mar	15-Nov	15-Feb	None
26	31-Mar	15-Nov	15-Feb	None

end_table

Appendix 2 The GeoPEARL_3.3.3 input file – Expert users

This appendix gives a listing of the GeoPEARL_3.3.3 input file. This file is intended to be used by expert users. Differences in the input file of GeoPEARL_3.3.3 compared with GeoPEARL_2.2.2 are set in bold face.

```
*-----
* GeoPEARL input file, generated by GeoPEARLGui
*
3 ModelVersion   Model version
3 GUIVersion    GUI version
3 DBVersion     Database version
*-----

*-----
* GeoPEARL control
*-----

* Directory structure
* The input directory is obtained from the model call.
Output          OutputDir          Output directory
..\..\SCHEMA~1  SchematisationDir    Spatial schematisation directory
..\..\Temp      PearlDir             Tmp directory for PEARLMODEL

* General control
IOMode_Full     IOMode               Screen output control
Low             PriorityClass         Priority class
SkipErrors     OptAppend            Append results (Yes|No|New)?
Yes            OptDelPloFiles      Should other files be removed (Yes|No)?
Yes            OptIrrigation        Simulate irrigation (Yes|No)?

* Timers - TimStart and TimEnd must be in range with dates in .met files
01-Jan-1901    TimStart             Start time of the simulation
31-Dec-1934    TimEnd              End time of simulation
6              InitYears           Number of years for initialization (0|10)

* Number of CPUs available for grid computing
1              NumCPU              Number of CPUs (1|-)
1              CPUID               Number of the current CPU (1|NumCPU)

*-----
* Reference to plot file and plots included in model run
* The plot files must be stored in the schematisation directory
*-----
Schematisation  Plots                Plot file (plo file - in plots dir)
Automatic       OptPlotList          Option: (Automatic|Manual|Generate_Only)

*-----
* If OptPlotList = Automatic
* Crop area database (unc file) must be stored in the schematisation directory
* For guidelines with respect to the selection of the number of zones:
* please read the manual
Schematisation  CropAreaDatabase     File with crop area per UC (unc file)
0.01            ThresholdArea (ha)   Threshold area (0|-)
250            NumZone              Number of zones
Rank            OptPlotSelection     Option: (Neighbour|Rank)

* Crops for which a registration is submitted. The model takes the sum of the
* crop areas of the individual crops. Make sure that the name is exactly equal
* to one of the names in the crop area database.

table Crops
11 FruitCulture
end_table
```

*-----
 * File with included plots - file must be in schematisation directory
PlotsIncluded **IncludedPlots** **File with plots to be included**
 *-----

*-----
 * SWAP missers - file must be put in schematisation directory
PlotsExcluded **ExcludedPlots** **File with SWAP missers**
 *-----

*-----
 * Compound and application information
 *-----

Substances CompoundProperties Compound properties
 Applications ApplicationSchemes Application schemes

*-----
 * Substances and application scheme. A run is made for each substance included
 * Column 1 : Pesticide code - must be included in CompoundProperties file
 * Column 2 : Application code - must be included in Applications file
 * Column 3+ : Compound codes included in run (first = the daughter)
 *-----

table Runs
 CMPCPF4 Persistentie_chlorpyrifos CPF4 TCP4
 end_table

*-----
 * Soil information (files must be stored in soil directory)
 * The soil file must be placed in the schematisation directory
 *-----

Schematisation SoilDatabase Soil database (sol file)

*-----
 * Crop information
 * The crop file must be placed in the schematisation directory
 *-----

Schematisation CropDatabase File with crop properties (crp file)
Schematisation **PloughingData** **File with ploughing dates (plg file)**

*-----
 * Information about meteo stations
 * The meteo files must be stored in the schematisation directory
 * Column 1: ID
 * Column 2: Latitude
 * Column 3: Altitude (m)
 * Column 4: Initial temperature (C)
 * Column 5: Option for potential evapotranspiration
 * ... Input : Reference evapotranspiration provided by user
 * ... Penman : Penman reference evapotranspiration
 * ... Makkink : Makkink reference evapotranspiration
 * ... PenmanMonteith : Penman Monteith evapotranspiration
 * Column 6: Reference to the meteo file (met file)
 *-----

table MeteoStations
 1 52 10 9.97 Input DeKooy
 2 52 10 9.97 Input Leeuwarden
 3 52 10 9.97 Input Eelde
 4 52 10 9.97 Input Hoorn
 5 52 10 9.97 Input Lelystad
 6 52 10 9.97 Input Dedemsvaart
 7 52 10 9.97 Input Naaldwijk
 8 52 10 9.97 Input DeBilt
 9 52 10 9.97 Input Winterswijk
 10 52 10 9.97 Input Andel
 11 52 10 9.97 Input Vlissingen
 12 52 10 9.97 Input Oudenbosch
 13 52 10 9.97 Input Gemert
 14 52 10 9.97 Input Venlo
 15 52 10 9.97 Input Beek
 end_table

```

*-----
* Local and regional groundwater system
* These files must be stored in the schematisation directory
Schematisation      GroundwaterSystem      Groundwater system (lbo file)
schematisation      DrainageSystem          Local drainage system (dra file)
*-----
* Output control data

Yes                OptScreen              Screen option (No|Swap_Only|Yes)
..\..\SCHEMA~1\Schematisation OutputControl          File with output data (ctr file)
Yes                PrintCumulatives      Print fluxes cumulative (Yes|No)
Fixed              OptZFoc               Option for ZFOC (Fixed|Variable)
1                  ZFoc                  (m) Depth of layer for balances (0.1|-)
0.05              ThiLayPer           (m) Evaluation depth for persistence
                               (0.01|-)

DaysFromSta       DateFormat             Format of dates in the output file
                               (DaysFromSta|DaysFrom1900|Years)
G12.4             RealFormat            Format of reals in the output file
Decade            OptDelTimPrn          Option for time step
                               (Day|Decade|Month|Year|Calculated|Other)
1                  DelTimPrn             (d) Print time step - only if option
                               is input (1.0|-)
Automatic          OptHyd                SWAP mode: (Automatic|OnLine|Only)
GeoPEARL          OptReport             (FOCUS|DutchRegistration|GeoPEARL) report
Yes              OptPersistency    Calculate persistency (Yes or No)
*-----
* SWAP control parameters

No                OptHysteresis          Simulate hysteresis (No|Yes)
1000000          MaxItSwa              Maximum number of iterations
                               (2|1000000)
0.005            ThetaTol              (m3.m-3) Tolerance for SWAP (1e-5|1e-2)
1E-5             DelTimSwaMin          (d) Minimum time step for SWAP
                               (1.e-8|0.1)
0.2              DelTimSwaMax          (d) Maximum time step for SWAP
                               (0.01|0.5)
1                  GWLTol                (m) Tolerance for groundwater level
                               (1e-7|1e2)
*-----
* End of file

```


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