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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This document was produced in accordance with the Quality Manual of the Statutory Research Tasks Unit for Nature & the Environment.

WOT Working Document 103 presents the findings of a research project implemented for and financed by the Ministry of Agriculture, Nature and Food Quality (LNV).
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Werkdocument 103
Wettelijke Onderzoekstaken Natuur & Milieu
Wageningen, oktober 2008
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's 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 platformTM 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 practices 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.
Additions and Changes to User’s 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 geopearl_3.3.3.exe. This archive is available at the download page of the PEARL website, which is at the address http://www.geopearl.pesticidemodels.eu.
• Figure 3, first step: Download geopearl_3.3.3.exe from the address http://www.geopearl.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.
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.
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

<table>
<thead>
<tr>
<th>Crop name</th>
<th>Number of plots for crop</th>
</tr>
</thead>
<tbody>
<tr>
<td>Potatoes</td>
<td>1043</td>
</tr>
<tr>
<td>Legumes</td>
<td>920</td>
</tr>
<tr>
<td>Fallow</td>
<td>1256</td>
</tr>
<tr>
<td>Cereals</td>
<td>1089</td>
</tr>
<tr>
<td>LeafVegetables</td>
<td>771</td>
</tr>
<tr>
<td>Floriculture</td>
<td>1009</td>
</tr>
</tbody>
</table>

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

Persistence output was based on a thickness layer of 0.05 meter

Overall persistence results:

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

Table 1: The output on the persistency of the substance at the predefined end points as included in the GeoPEARL report.

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

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 ‘geopearl_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 platformTM 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

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
<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>15-Apr</td>
<td>15-Nov</td>
<td>15-Feb</td>
<td>None</td>
</tr>
<tr>
<td>21</td>
<td>31-Mar</td>
<td>15-Nov</td>
<td>15-Feb</td>
<td>None</td>
</tr>
<tr>
<td>22</td>
<td>01-Mar</td>
<td>15-Dec</td>
<td>15-Feb</td>
<td>None</td>
</tr>
<tr>
<td>23</td>
<td>15-Aug</td>
<td>15-Nov</td>
<td>15-Feb</td>
<td>None</td>
</tr>
<tr>
<td>24</td>
<td>31-Mar</td>
<td>15-Nov</td>
<td>15-Feb</td>
<td>None</td>
</tr>
<tr>
<td>25</td>
<td>31-Mar</td>
<td>15-Nov</td>
<td>15-Feb</td>
<td>None</td>
</tr>
<tr>
<td>26</td>
<td>31-Mar</td>
<td>15-Nov</td>
<td>15-Feb</td>
<td>None</td>
</tr>
</tbody>
</table>

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

Documentation update for GeoPEARL_3.3.3 19
* File with included plots - file must be in schematisation directory

<table>
<thead>
<tr>
<th>PlotsIncluded</th>
<th>IncludedPlots</th>
<th>File with plots to be included</th>
</tr>
</thead>
</table>

* SWAP missers - file must be put in schematisation directory

<table>
<thead>
<tr>
<th>PlotsExcluded</th>
<th>ExcludedPlots</th>
<th>File with SWAP missers</th>
</tr>
</thead>
</table>

* Compound and application information

<table>
<thead>
<tr>
<th>Substances</th>
<th>CompoundProperties</th>
<th>Compound properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>Applications</td>
<td>ApplicationSchemes</td>
<td>Application schemes</td>
</tr>
</tbody>
</table>

* 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

<table>
<thead>
<tr>
<th>Schematisation</th>
<th>SoilDatabase</th>
<th>Soil database (sol file)</th>
</tr>
</thead>
</table>

* Crop information

* The crop file must be placed in the schematisation directory

<table>
<thead>
<tr>
<th>Schematisation</th>
<th>CropDatabase</th>
<th>File with crop properties (crp file)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Schematisation</td>
<td>PloughingData</td>
<td>File with ploughing dates (plg file)</td>
</tr>
</tbody>
</table>

* 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 Belde
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 DeSilt
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

<table>
<thead>
<tr>
<th>Schematisation</th>
<th>GroundwaterSystem</th>
<th>Groundwater system (lbo file)</th>
</tr>
</thead>
<tbody>
<tr>
<td>schematisation</td>
<td>DrainageSystem</td>
<td>Local drainage system (dra file)</td>
</tr>
</tbody>
</table>

*-------------------------------------------------------------------------------

* Output control data

| Yes                      | OptScreen        | Screen option (No|Swap.Only|Yes) |
|--------------------------|------------------|------------------|
| \..\..\SHEMA~1\Schematisation | OutputControl | File with output data (ctr file) |
| Fixed                    | OptZFoc         | Option for ZFOC (Fixed|Variable) |
| 1                        | ZFoc            | Depth of layer for balances (0.1|-) |
| ThiLayPer                |                  | 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       | 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

| Yes                      | OptHysteresis | Simulate hysteresis (No|Yes) |
|--------------------------|---------------|-----------------------|
| 10000000                  | MaxItSwa      | Maximum number of iterations (2|1000000) |
| 0.005                    | ThetaTol      | Tolerance for SWAP (1e-5|1e-2) |
| 1E-5                     | DelTimSwaMin  | Minimum time step for SWAP (1.e-8|0.1) |
| 0.2                      | DelTimSwaMax  | Maximum time step for SWAP (0.01|0.5) |
| 1                        | GWLTol        | Tolerance for groundwater level (1e-7|1e2) |

*-------------------------------------------------------------------------------

* End of file

Documentation update for GeoPEARL_3.3.3 21
WOT-onderzoek

Verschenen documenten in de reeks Werkdocumenten van de Wettelijke Onderzoekstaken Natuur & Milieu vanaf 2006

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2006

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27 Jaarrapportage 2005. WOT-04-501 Kennisbasis
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2007


Documentation update for GeoPEARL_3.3.3 23