

User manual for GeoPEARL version 4.4.4

F. van den Berg, A. Tiktak, D.W.G. van Kraalingen, J.G. Groenwold & J.J.T.I. Boesten

| WOt-technical report 139



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User manual for GeoPEARL version 4.4.4

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User manual for GeoPEARL version 4.4.4

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Abstract

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In the Dutch Decision Tree for the evaluation of the leaching potential of pesticides, the GeoPEARL model is used to calculate the 90th spatial percentile of the median leaching concentration in time at a depth of 1.0 m. This user manual describes the use of the graphical user interface of this version. In addition a description of the input and output files is given which helps the user to use the GeoPEARL model without the interface.

Keywords: crop protection product, Dutch decision tree, groundwater, leaching, pesticide

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Preface

This manual has been prepared to support the user of the new version of GeoPEARL. In this version, the organic matter contents as included in the soil schematisation of the Netherlands has been derived from the new soil organic matter map for the Netherlands. This new maps was necessary, because the soil organic matter contents in arable soils as included in the old soil schematisation were about a factor 1.5 to 2 too high. Other improvements include the option to use multiple cores for the calculations of GeoPEARL.

The GeoPEARL database of this version no longer contains substance specific data. To edit, store and archive these data a separate application has been developed, i.e. SPIN. The new version of GeoPEARL is coupled to SPIN versions 3.3.

Summary

In 2004, the Netherlands have adopted a new decision tree for the evaluation of the leaching potential of pesticides. In this evaluation procedure, the median leaching concentration over a period of 20 years of a pesticide or its relevant metabolites at 1.0 m depth should not exceed the drinking water limit of 0.1 µg/L within 90% of the area of use of the pesticide. To facilitate the calculation of this target value, the spatially-distributed model GeoPEARL has been developed. The first version of this model, i.e. GeoPEARL 1.1.1 has been released in 2004 in support of the introduction of the new decision tree. Since the introduction of this first version two updates have been released, GeoPEARL 2.2.2 (2006) and GeoPEARL 3.3.3. The latter version contains an option to select areas in which the top soil has specific properties, for example to exclude areas with a sandy topsoil.

In 2012 an error was found in the soil organic matter content of arable soils. This content in arable soils as introduced in the soil schematisation of the Netherlands as used by GeoPEARL was about 1.5 to 2 times higher than in reality. Therefore, a new soil organic matter map has been prepared for the Netherlands and this has been implemented in the soil schematisation of a new version for GeoPEARL, i.e. GeoPEARL 4.4.4

This report gives a guidance on the use of the new GeoPEARL 4.4.4 version. The GeoPEARL software package consists of a set of computation kernels, a Graphical User Interface and a database with the data on the spatial schematisation of the Netherlands to be used for the groundwater leaching assessments. The GeoPEARL model can be used with or without the Graphical User Interface. The manual describes both options. Using the schematisation data contained in the GeoPEARL database, the results of assessments obtained with or without the user interface are the same.

Samenvatting

In 2004 is een nieuwe beslisboom van kracht geworden om het risico van uitspoeling van gewasbeschermingsmiddelen te evalueren. In deze evaluatieprocedure mag de mediane uitspoelconcentratie van een pesticide of een relevante metaboliet over een periode van 20 jaar op een diepte van 1,0 m in 90% van het gebruiksareaal van het middel niet hoger zijn dan het drinkwater criterium van 0,1 µg/L. Om de berekening van deze doelgrootte te faciliteren is het ruimtelijk verdeelde model GeoPEARL ontwikkeld. GeoPEARL versie 1.1.1 is in 2004 uitgebracht om het gebruik van de nieuwe beslisboom voor uitspoeling te ondersteunen. Sinds de introductie van deze eerste versie zijn in de loop van de tijd twee updates uitgebracht: GeoPEARL 2.2.2 (2006) en GeoPEARL 3.3.3 (2008). De laatste versie biedt de mogelijkheid om gebieden te selecteren waarin de bovengrond specifieke eigenschappen heeft, bijvoorbeeld om gebieden uit te sluiten met een zandbovengrond.

In 2012 werd een fout geconstateerd in het organische-stofgehalte in akkerlandgronden. Het gehalte aan organische stof in akkerlandgronden, zoals dat opgenomen was in de bodemschematisatie voor Nederland in GeoPEARL, was ongeveer een factor 1,5 à 2 te hoog. Daarom is er een nieuwe organische-stofkaart gemaakt voor Nederland en deze is geïmplementeerd in de schematisatie van de nieuwe versie van GeoPEARL.

Dit rapport biedt ondersteuning bij het gebruik van de nieuwe GeoPEARL 4.4.4 versie. Het softwarepakket bevat een set rekenkernels, een gebruikersinterface en een database met de gegevens van de ruimtelijke schematisatie van Nederland die gebruikt wordt voor de risico-evaluaties voor uitspoeling naar het grondwater. Het model GeoPEARL kan zowel met als zonder het gebruikersinterface toegepast worden. Bij gebruik van de schematisatiegegevens zoals die zijn opgenomen in de database, is er geen verschil in uitkomsten in de evaluaties met of zonder het interface.

1 Introduction

In 2004, the Netherlands have adopted a new decision tree for the evaluation of the leaching potential of pesticides. In this decision tree, it is evaluated whether the concentration in groundwater exceeds the EU drinking water limit, which is 0.1 µg/L. A spatially distributed pesticide leaching model, GeoPEARL, has been developed. GeoPEARL calculates the leaching of a pesticide and its metabolites to the uppermost groundwater for the area of use. The target output for the Dutch pesticide registration procedure is the 90th areal percentile of the median leaching concentration over a period of 20 years. Further background information on the new decision tree on leaching can be found in RIVM report 601450019 (Van der Linden *et al.*, 2004).

In 2012 an error was found in the soil organic matter content of arable soils as used in the soil schematisation of GeoPEARL. The organic matter content in arable soils was found to about 1.5 to 2 times higher than in reality. Therefore, a new soil organic matter map has been prepared for the Netherlands and this has been implemented in the soil schematisation of a new version for GeoPEARL, i.e. GeoPEARL 4.4.4. This implementation and its consequences for the decision tree for the assessment of leaching to groundwater is described in Van den Berg *et al.* (2017).

This report contains a user-manual of GeoPEARL 4.4.4. Background information on GeoPEARL can be found in the earlier RIVM report 716601007 (Tiktak *et al.*, 2003). The new version of the GeoPEARL database does no longer contain the data on the physico-chemical properties of the compound. Instead, the new GeoPEARL version is coupled to SPIN (Substance PlugIN) version 3.3 to enter, edit or archive all substance data needed for a GeoPEARL assessment. More information on the SPIN application and as well as guidance to derive values for substance input parameters can be found in the SPIN Manual (Van Kraalingen *et al.*, 2019, i.v.). A detailed description of the processes considered in the PEARL model is presented by Van den Berg *et al.* (2016).

The manual consists of two parts. In Chapter 2, the Graphical User Interface is described. The Graphical User Interface gives easy access to the most important components of GeoPEARL, like the generation of input files, model execution, output processing and generation of the most important output maps and tables. Most users will use the GUI version of GeoPEARL only.

Chapter 3 contains a description of the command line version of GeoPEARL. The command line version of GeoPEARL is more flexible, but is also more difficult to use. Reasons to use the command line version of GeoPEARL may be:

- implementation of GeoPEARL on a grid computing system;
- use of a different spatial schematization, so that the model can be used for other countries.

The command-line version of GeoPEARL should only be used by experienced modellers. In contrast to the GUI version, the user can change all input parameters in the GeoPEARL input file.

Compatibility

GeoPEARL version 4.4.4 is not compatible with the previous versions of GeoPEARL, since the substance related data have been taken out from the database and have been transferred to a separate application SPIN, that has to be used to enter, edit and archive properties of the substances for which the GeoPEARL model is to be applied.

For data on substances and application schemes as defined in GeoPEARL 3.3.3, GeoPEARL 4.4.4 has the option to import these data into the GeoPEARL 4.4.4 database. This import procedure is described in Section 2.4.

2 User's guide GeoPEARL User Interface

2.1 General

This chapter gives an overview of the GeoPEARL user interface, which is an integrated environment for data storage and data retrieval, model control and viewing the output data (Figure 1). The user communicates with the GeoPEARL modelling system through the graphical user interface. This interface is linked with a relational database. It also generates the input files for the GeoPEARL executable. GeoPEARL in its turn calls the PEARL model. It does so for each unique combination of soil type, climate district, etc. These unique combinations are called plots. The output of GeoPEARL is transferred back to the user interface, from where it is stored in the database.

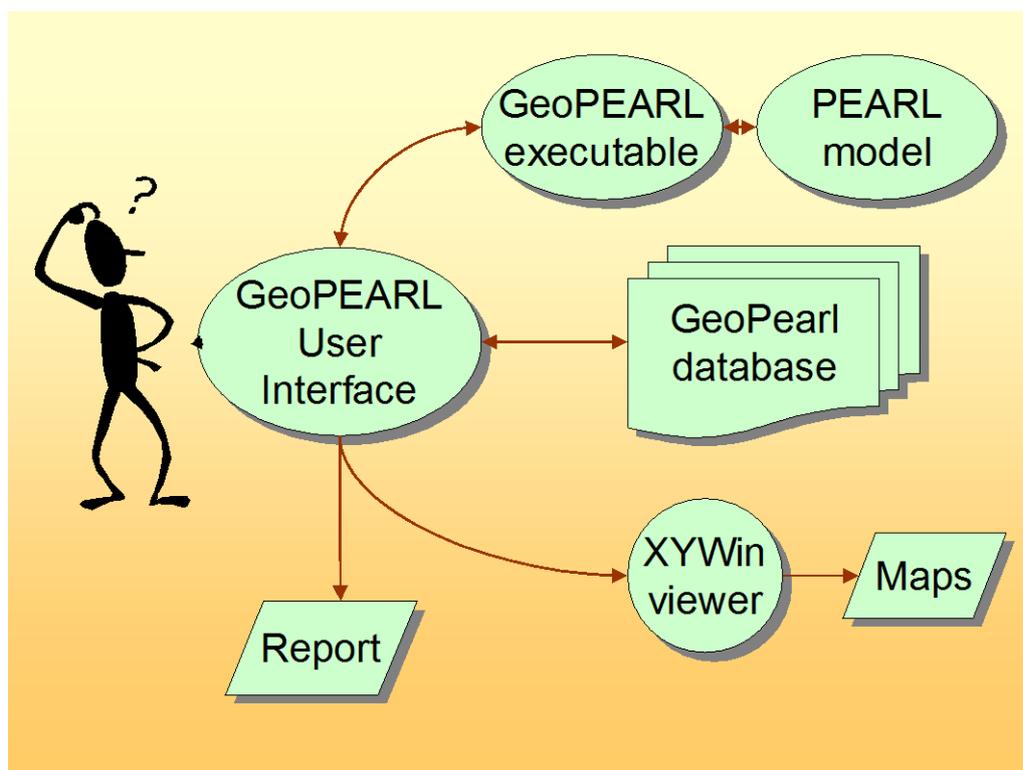


Figure 1 Overview of the GeoPEARL modelling system

With the user interface, the following tasks can be carried out:

- organize and edit application data;
- access the standardized model runs, which should be used for the Dutch pesticide registration procedure;
- control the model;
- view maps of major input variables;
- run the model;
- display a summary report, containing percentiles of the leaching concentration;
- display output maps;
- generate graphics files, which can be imported in (for example) Word.

2.2 Database structure

In order to organize the data efficiently, the data are stored in a relational database. Figure 2 shows how the data are organized in this database. As shown in later sections of this manual, the screens of the GeoPEARL GUI have the same set-up as the database.

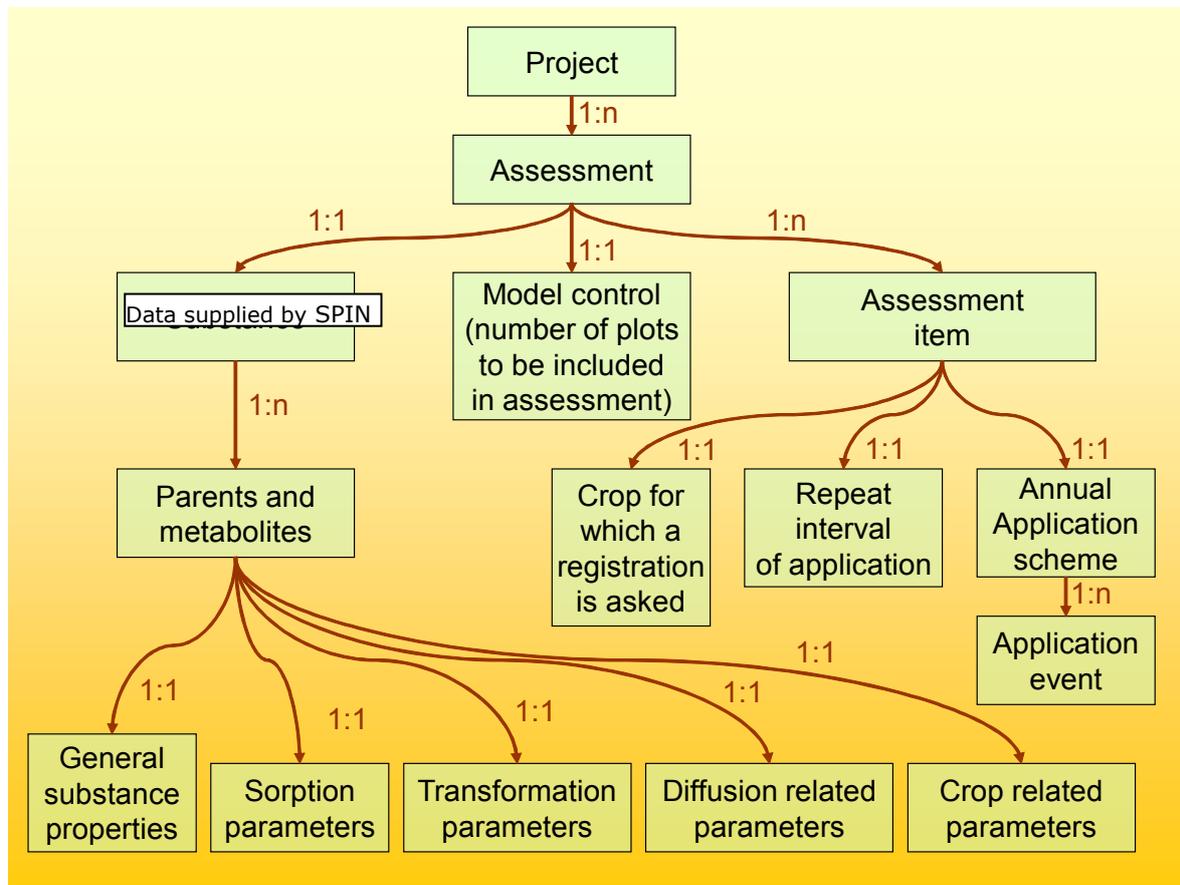


Figure 2 Overview of the GeoPEARL database. Only parameters that can be changed by the user are included in the diagram.

The GeoPEARL database has a hierarchy. The highest level of the database is the project level. Here, the user can group several assessments, based on a common criterion (e.g. all assessments related to a particular registration dossier). The second highest level is the assessment level. An assessment is the basic entity in GeoPEARL. A GeoPEARL assessment is carried out for a single substance, but may consist of several so-called assessment items. Assessment items are combinations of a crop for which a registration is asked and an application scheme. This implies that different crops can have different application schemes.

The GeoPEARL database also contains the data of the spatial schematization, such as soil type, climate district and drainage system. These data are locked and cannot be changed by the user; for this reason they are not shown in Figure 2.

Assessments are the central entity in the GeoPEARL user interface. For each assessment, the interface calculates the area of usage and summary statistics like the 90th percentile of the leaching concentration at the area of usage, the latter being the target variable in the Dutch registration procedure (see Tiktak *et al.*, 2003).

As mentioned above, an assessment can consist of various items. For example, a company might wish to request a registration for maize, potatoes and cereals. In that case, the assessment must contain three items. For each item, a GeoPEARL run is carried out and the 90th percentile of the leaching concentration is calculated for the total area of maize, potatoes and cereals.

2.3 Installation of the GeoPEARL User Interface

Before using GeoPEARL, you have to install the model. The software package is contained in a zip file. After unzipping this file, the user can start the installation procedure by clicking on the exe file extracted from the zip file. Next the user has to follow the on-screen instructions. An overview of the installation procedure is shown in Figure 3.

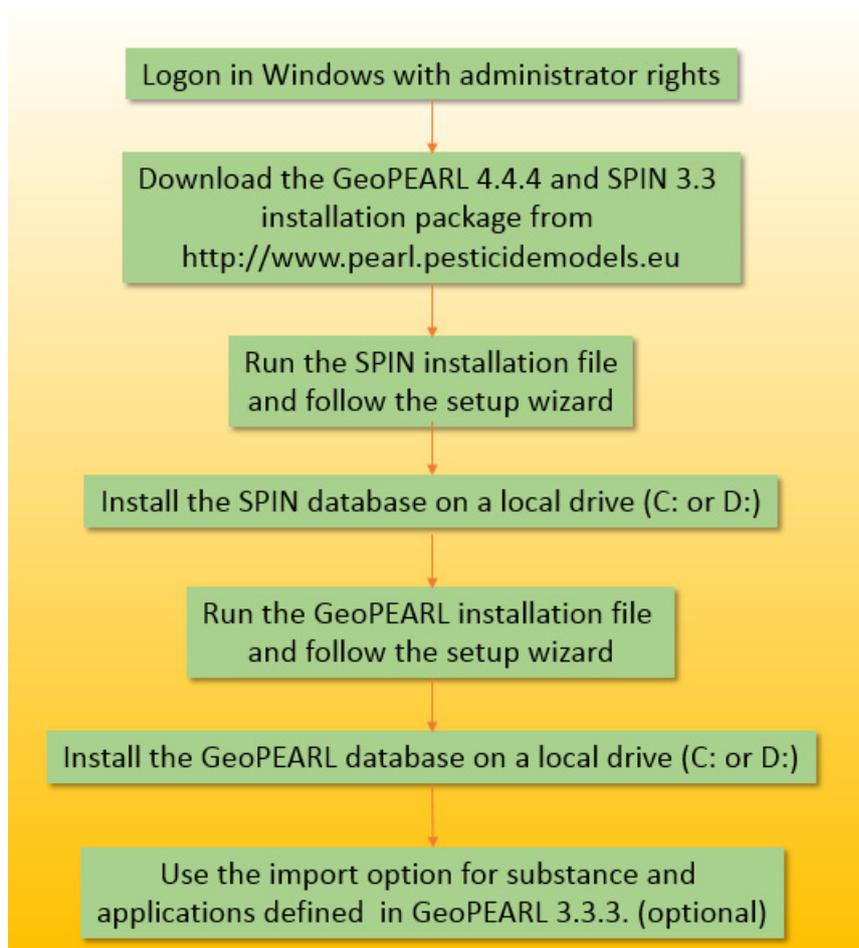


Figure 3 Installation procedure of GeoPEARL 4.4.4 and importing data from GeoPEARL 3.3.3 database and SPIN 3.3.

During the setup procedure, you will see the license agreement and the contents of the file `ReadmeDuringInstallation.rtf`. We strongly recommend reading the information in these files; in particular in relation to the selection of the installation folder for the database.

You should be aware of the following:

- the operation system must be Windows 7 or higher. Windows XP and Windows Vista are no longer supported by the PEARL team.
- you must have full administration rights during the installation procedure and during the first time that you start using GeoPEARL. If you don't have full administration rights, logon to your computer with a user name that has administrator rights. It may be necessary to contact your systems operator.

2.4 Import data from GeoPEARL 3.3.3

For user defined substances and applications used in GeoPEARL 3.3.3, there is an import option available in the menu. This is shown in Figure 4.

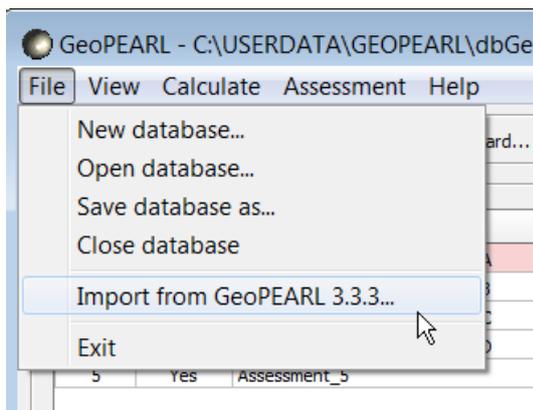


Figure 4 Import option for substances and applications from the GeoPEARL 3.3.3 database into the GeoPEARL 4.4.4 database.

Please note that this option only works if GeoPEARL 3.3.3 has been installed and is working properly on the machine on which the new version has been installed. This warning is also shown on the screen after selecting this option from the main form of GeoPEARL 4.4.4 (see Figure 5).

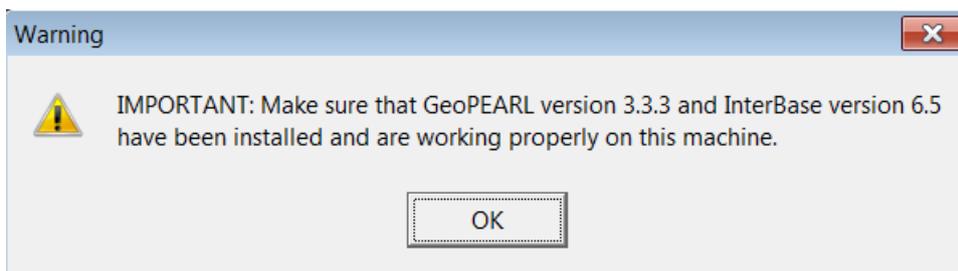


Figure 5 Notification before import procedure will start.

After clicking on 'OK' the database of GeoPEARL 3.3.3 is coupled automatically. Then the user can start the import wizard for import of data on substances or application schemes. These options are shown in Figure 6.

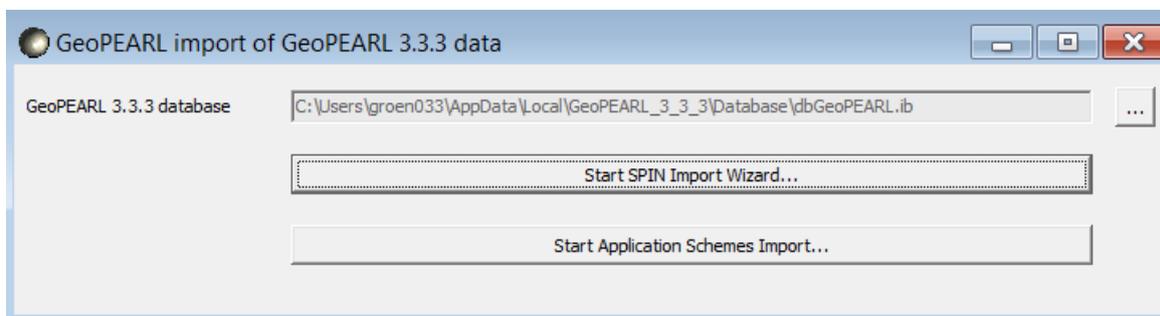


Figure 6 Select which data should be imported from GeoPEARL 3.3.3.

After the import procedure has been started, a log process is displayed on the screen about the status of the import (see Figure 7).

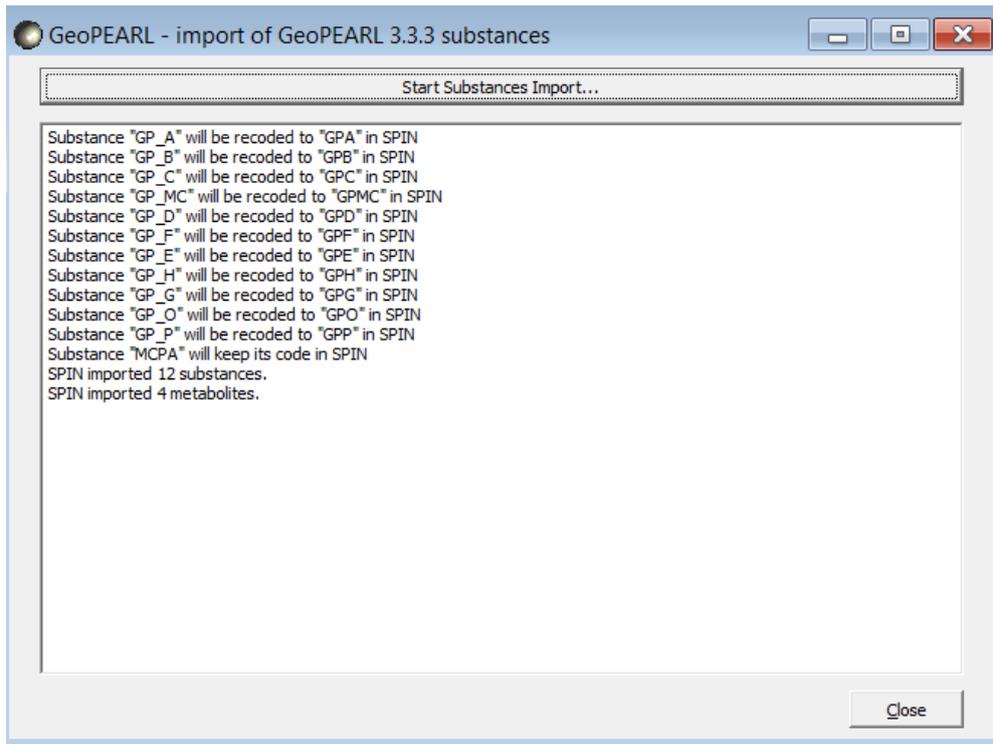


Figure 7 Import log of imported substances.

The same procedure can be followed for the application schemes. After this procedure has been started, a log process is displayed on the screen about the status of the import, which is shown in Figure 8.

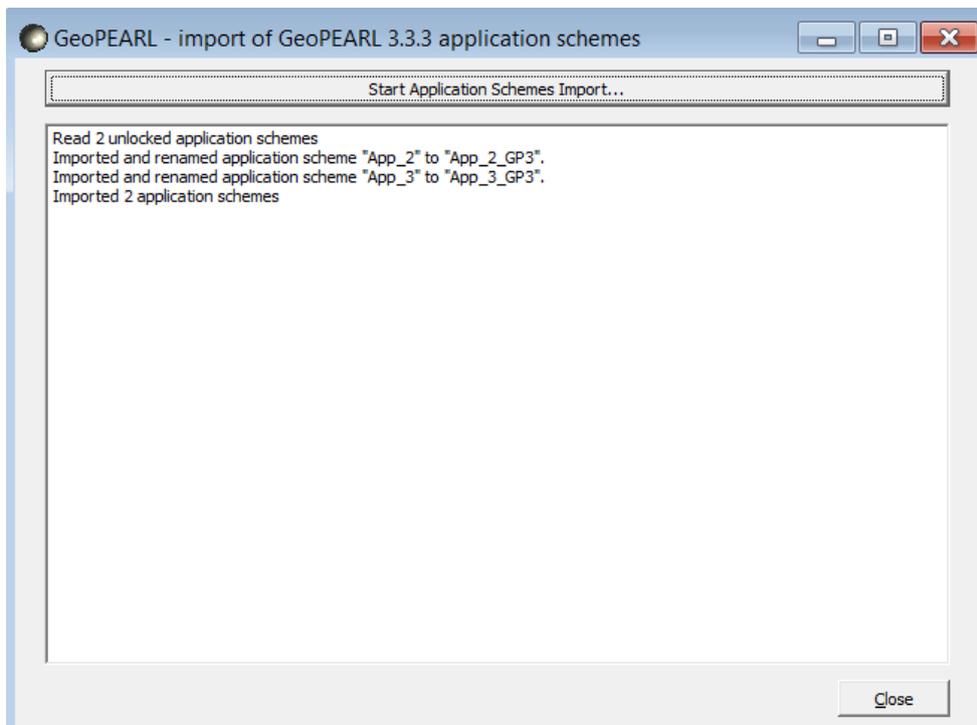


Figure 8 Import log of imported application schemes.

2.5 Getting started with the GeoPEARL User Interface

The user should first define the building blocks of an assessment (see Figure 2). This implies that first the substances and application schemes must be defined. This comes down to the following steps (Figure 9):

- Define or edit substances. Physico-chemical properties, sorption parameters, transformation parameters and parameters for interaction with plants should be defined for the substance and all its metabolites to be included in the calculations. Please take notice that the substance data are stored in a separate database SPIN (see SPIN manual, Van Kraalingen *et al.*, 2019; i.v.).
- Define or edit the application schemes. As each assessment item may have its own application scheme, several assessment schemes may be required (see Section 2.2).
- Use the assessment wizard to define an assessment.
- Check the settings within the assessment and correct if necessary.
- Perform the calculations by selecting the assessments and push the calculate button to start the calculations.
- Assess the results.

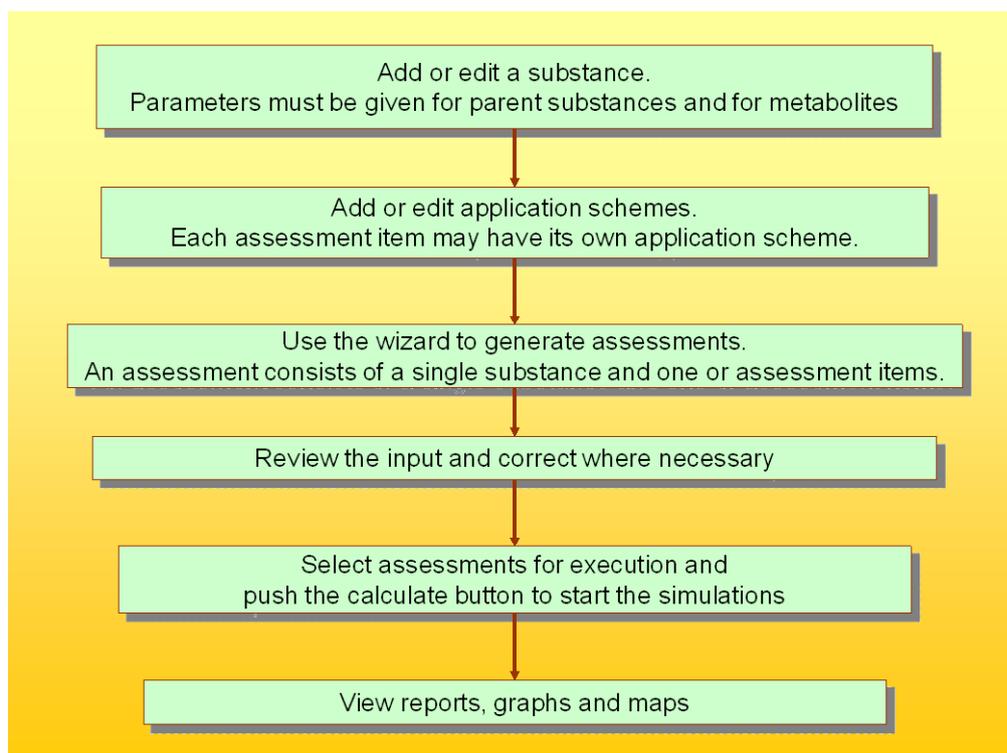


Figure 9 Major steps of a GeoPEARL assessment

The five steps are elaborated in a little bit more detail below.

Step 1. Add or edit a substance

The substances properties are now handled in the SPIN application. For adding and editing substances to be used in GeoPEARL, see the SPIN Manual (Van Kraalingen *et al.*, 2019; i.v.).

Step 2. Add or edit one or more application scheme(s)

In GeoPEARL it is not possible to specify pesticide applications relative to crop emergence (so-called relative applications). The reason is that in GeoPEARL the crop emergence dates are part of a fixed spatial schematization, which cannot be manipulated by the user.

To create a new application scheme, do the following:

- From the main screen, select View Application Schemes from the drop down menu at the top to go to the Application Schemes form.

-
- Click + on the navigator of the Application Schemes box (left-hand side of form) to add an application scheme.
 - Fill in a unique code and a name.
 - Click + on the navigator of the Applications box to add an application.
 - Select the type of application and enter the other application parameters.
 - Repeat the last two steps if a substance is applied multiple times a year.
 - Click close when all applications have been added to return to the main scheme.

More information on editing application schemes can be found in Section 2.9.

Step 3. Run the wizard

Press the Wizard button on the main screen to start a GeoPEARL assessment.

- Specify a name, the spatial detail wanted (i.e. the number of plots) and the substance for which GeoPEARL should be run. In order to get a reliable estimate of the 90th percentile of the leaching concentration, the number of plots should be at least 250. When done, select Next.
- Select a crop, an application scheme and the application interval. Then select Add.
- Repeat the last step for all combinations of crops and application schemes to be included in the assessment.
- Select Finish to go back to the main form.

Step 4. Refinement

GeoPEARL has now created an assessment. This assessment has already been selected for execution. Before actually running the model, it is advisable to review the most important model inputs. Where necessary, changes can be made.

Step 5. Running GeoPEARL

Press the Calculate button on the main screen to actually run the model. The actual runtime for the model is hard to predict, as it depends on the hardware, the number of assessment items and the number of plots that you have included. Anyhow, a typical GeoPEARL assessment for 250 plots will take a few hours if running on a single core. We therefore recommend to use state-of-the-art hardware only. When an assessment is ready, you will see the 'Results' column changing to Yes. If something has gone wrong, the Error button becomes active.

Step 6. Review results

- Press the Report button to review the summary report. This report contains, amongst others, the 90th percentile of the leaching concentration at the area of use, which is the target variable in the Dutch registration procedure.
- Press the Graphs and Maps button to view maps of the leaching concentration, maps of terms of the substances balances, etcetera.

2.6 The projects form

The project form can be accessed from the main screen (see Section 2.7). The projects form allows you to organize your data. Existing projects can be selected in the browse box (upper part of form). The navigator allows you to create or delete projects. An appropriate description can be added in the edit part.

2.7 The main screen

The main form (Figure 10) is the central point from where you can access the different tables of the database, run the wizard and view model inputs and model outputs. Most of the steps described in Section 2.5 will be carried out from the main screen. You can use buttons, the main menu or shortcut keys to navigate through the GeoPEARL User Interface.

The main menu

The main menu can be used for easy access to various parts of the GeoPEARL user interface:

- Use File submenu to open another database (Key combination: Alt-F-O) or to exit GeoPEARL (Alt-F-X).
- Use the View submenu to directly jump to the projects form (Alt-V-P), the substances form (Alt-V-S) or the applications form (Alt-V-A).
- Use the Calculate submenu to start the calculations (Alt-C-C) or to select/unselect all assessments for execution.
- Use the Assessment submenu to run the Wizard (Alt-A-W), to move an assessment to another project (Alt-A-M) or to archive an assessment (Alt-A-A).
- Use the Help submenu to find model documentation, the GeoPEARL website and Help desk information.

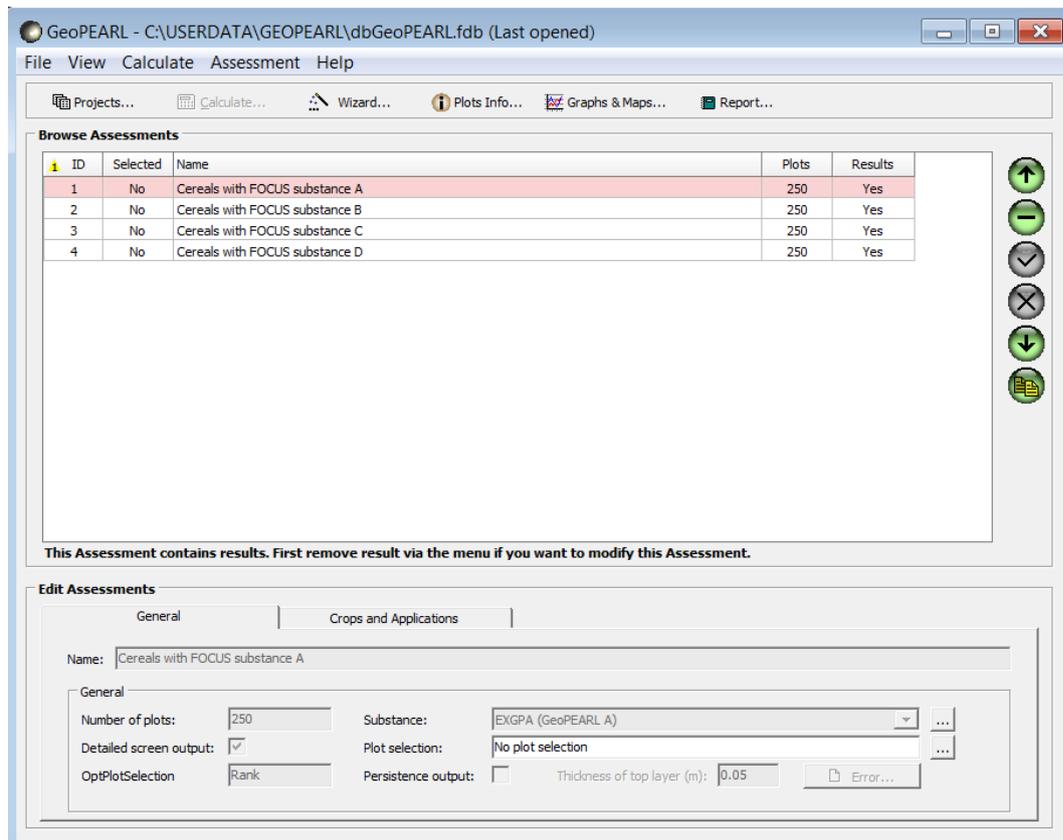


Figure 10 The main form of the GeoPEARL User Interface.

The lower part of the screen gives information on browsed assessments. Furthermore you can indicate here the amount of information that will be shown on the screen during the calculation. When you check 'detailed screen output' more information will be shown on the screen during the calculations. This will, however, slow down the simulations.

2.8 Editing substances

The substances form is accessible from the main form of GeoPEARL. GeoPEARL can simulate the fate of a parent pesticide and its formation products (metabolites) in soil. This implies that both the properties of the individual compounds, and the transformation scheme have to be parameterized. Both are accessible from the pesticides form. Input must be carried out in the following order:

- Definition of the properties of the individual compounds.
- Definition of the transformation scheme. This step can be ignored if only one compound is simulated.

At least one compound, the parent compound, must be introduced. This compound will be applied and/or deposited.

2.9 Editing application schemes

Application schemes

The application schemes form is accessible from the main menu of the main screen (View-Application Schemes). The entire events scheme can be repeated annually, biennially or triennially using the 'application interval' option at the main screen.

Event schemes (Events) can be added with the + button of the navigator. You can also copy an existing event scheme. Event schemes should be given a *unique* code for reference and a description. Use the 'Events' button to define the individual events.

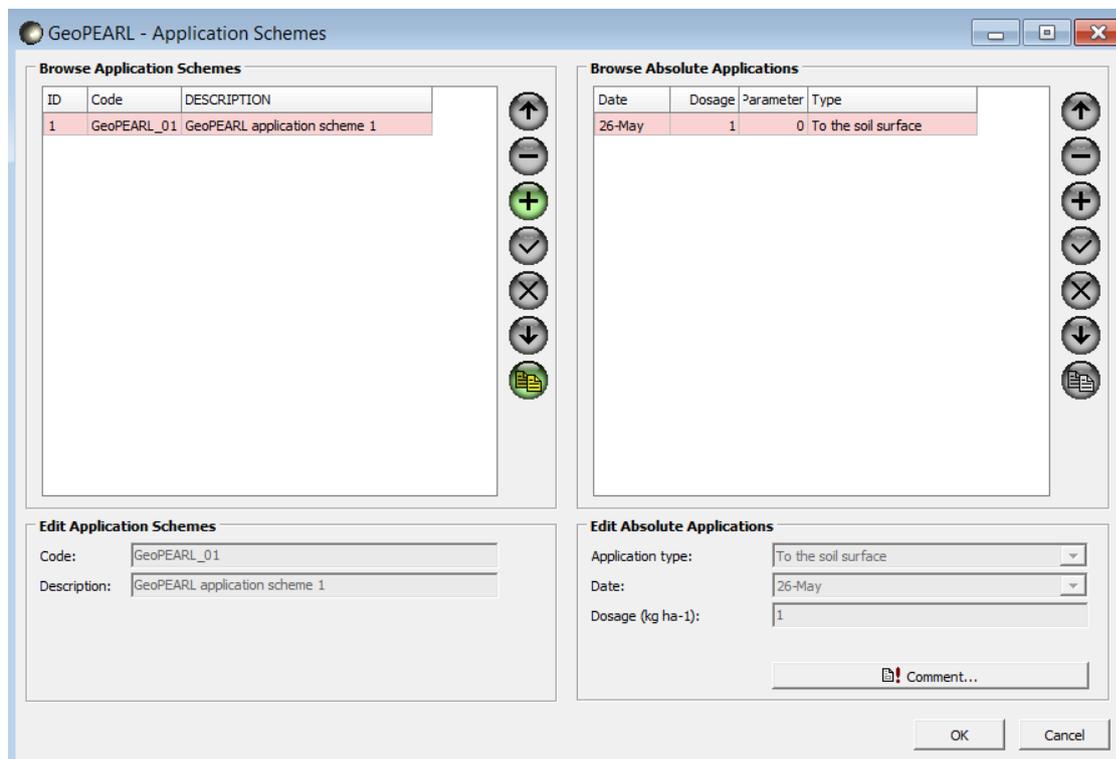


Figure 11 The application schemes form.

Applications

Add a new event with the + button of the navigator or copy an existing event (Figure 11). In the lower half of the screen, the event has to be further defined. First define the application type: 'application to the soil surface' (AppSolSur), 'injection' (AppSolInj), 'incorporation' (AppSolTil) or 'application to the crop canopy, interception fraction supplied by the user' (AppCrpUssr). Then enter the date and the dosage, normal date format (dd-MMM) can be used. The year is not required as GeoPEARL always repeats the entire application scheme annually, biennially or triennially. In the case of injection or incorporation, you must additionally supply the incorporation or injection depth.

2.10 Composing an assessment with the Assessment Wizard

As described in Section 2.2, an assessment is the basic entity of GeoPEARL. An assessment is carried out for a single substance and for one or more assessment items, which are combinations of crops and application schemes. Assessments are composed using the Wizard button on the main screen. You can compose an assessment after the substance and the application schemes that you want to use in your GeoPEARL calculations are defined. After selecting the assessment wizard, the following screen appears (Figure 12).

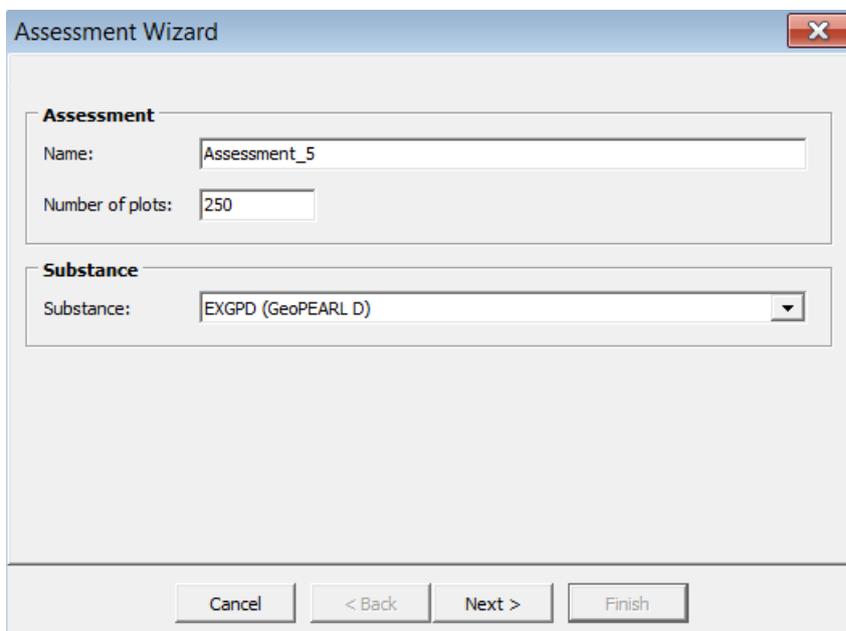


Figure 12 First screen of the assessment wizard.

Type the name of the assessment and define the number of plots to be included in the assessment. You can enter a number between 2 and 6405. However, for a reliable calculation of the 90th percentile of the leaching concentration, at least 250 plots should be used (see Van der Linden *et al.* 2004, Appendix 4). Use a lower number only for test runs. If the given number of plots is larger than the number of plots available for a certain crop, then GeoPEARL calculates for the maximum number available.

Subsequently select a substance (defined earlier) and click the Next button. The screen shown in Figure 13 will appear. Select a crop, an application scheme (defined earlier) and a repeat interval for the application scheme (i.e. annually, biennially or triennially) and click the Add button. Repeat this step for every crop you want to be included in the assessment. It is not possible to select a crop twice (with different application schemes) in a single assessment. Press the Finish button after having selected all combinations for the assessment. You return to the main screen, from where you can work further.

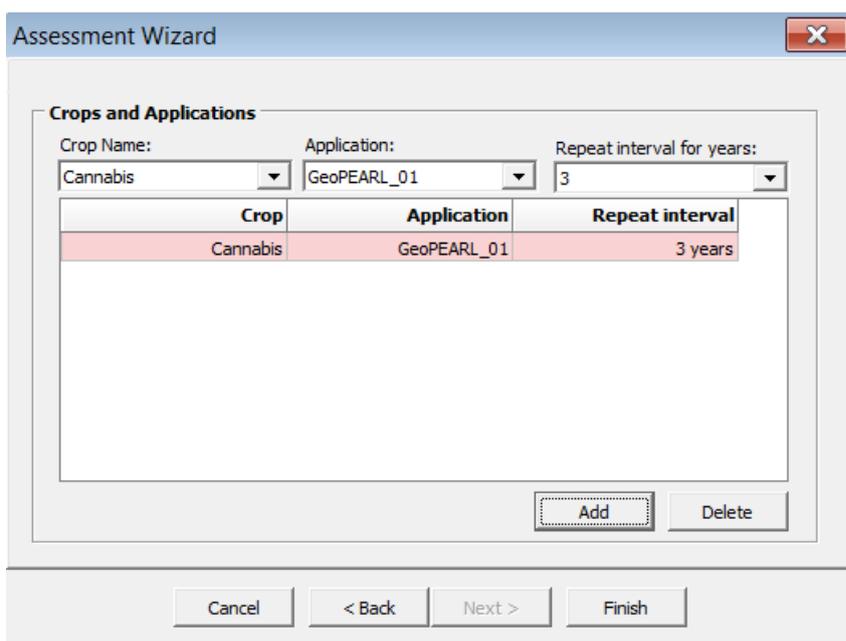


Figure 13 Second screen of the assessment wizard.

Crops are used in GeoPEARL to identify the area of use of a plant protection product. You can choose from 26 entries. Most of the entries consist of a single crop or a crop group and it will be quite clear from the name what is meant. For example, the entry 'potatoes' stands for all potato crops, so including seed potatoes, starch potatoes and potatoes for consumption. The following entries need explanation:

- Fallow: agricultural area, indicated not to be used for production of crops for some period.
- Plants for commercial purposes: caraway, flax, poppy seed and rapeseed.
- Remaining agricultural crops: crops not identified by other entries, usually these crops individually have an acreage up to a few hundred hectares.
- Total agricultural area: area of all crops (including fallow) together.
- Total non-urban area: total non-built-up area, i.e. agricultural area and nature area.

The 24 crops / crop groups (including fallow) can be combined in an assessment. For example, it is possible to select both sugar beets and potatoes in an assessment. It is, however, impossible to combine individual crops with the total agricultural area or the non-urban area; this would lead to overlap in areas. Likewise it is impossible to combine the agricultural area and the total area.

2.11 Checking assessment definitions

Back at the main screen you can check the definitions of the assessments. If necessary, you can make changes immediately by editing an assessment in the main screen. The main screen gives an overview of the most important items of the assessment, in two tabs. All the assessment items can be changed in the respective tabs.

2.12 Running the model

An assessment can be selected for execution by double clicking the respective assessment. Multiple assessments can be selected; all selected assessments are executed by pressing the 'Calculate' button on the main screen. In the main menu, you can select or deselect all assessments in a project at once (menu item Calculate).

First you can choose how to run the assessment, see Figure 14. There are three options for calculations:

- Normal window: the calculation process is shown on top of the main screen.
- Minimized window: the progress of the calculation process is shown in a window that can be shown on top of the main screen if the user clicks on the GeoPEARL item on the windows task bar.
- Hidden: no window can be shown; the calculations run as a process in the background.

The default option to execute the assessments is 'Minimized'.

There is an option to distribute the GeoPEARL 4.4.4. model runs over multiple cores. The interface checks the number of available cores in the computers and keeps 1 core for other Windows tasks. The user can select in the range of available cores.

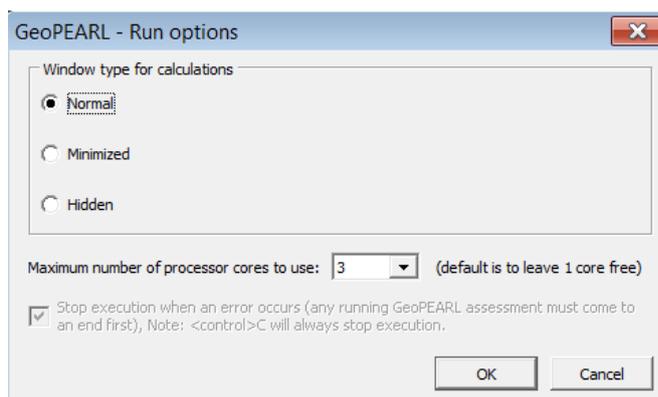


Figure 14 Run options for running the GeoPEARL model

After starting the calculations, a GeoPEARL progress screen will appear, which is shown in Figure 15. This screen roughly indicates the progress of the execution at the bottom of the screen.

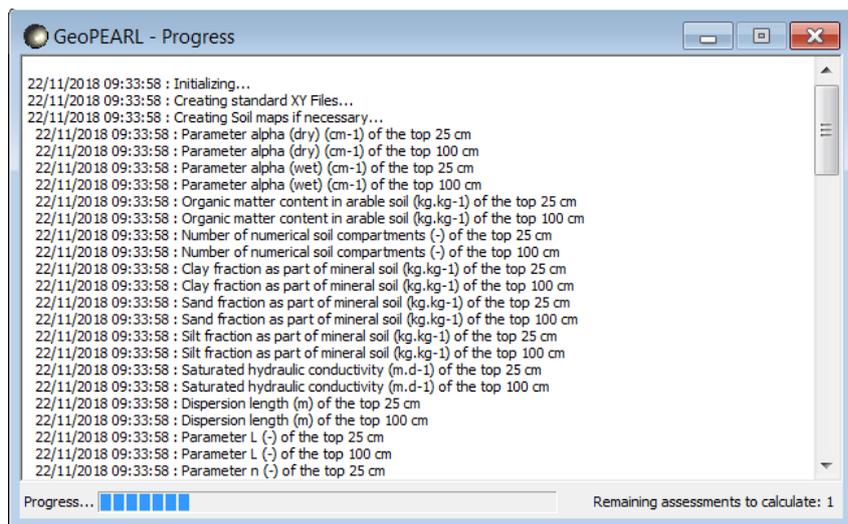


Figure 15 Screen indicating the progress of model execution.

2.13 Reports showing the target variable for registration

When GeoPEARL has terminated successfully, you will see that the Results column is set to Yes. Also, the Reports button will become highlighted. You can use this button to view a summary report, which shows the 90th percentile of the leaching concentration for the area of usage. As described Section 2.10, this area is represented by the total area of the crops selected when composing an assessment (see Tiktak *et al*, 2003, Section 2.5). The reports contain information on the leaching concentration of all substances, including metabolites.

The 90th percentile of the leaching concentration is calculated in a number of steps:

1. For each plot average leaching concentrations are calculated for 20 calculation periods. The length of the calculation periods is one year in the case of annual applications, two years in the case of biennial applications and three years in the case of triennial applications (conform FOCUS, 2000).
2. From these 20 values, the median value is taken. The result is considered the leaching concentration of a plot.
3. The 90th percentile in space is calculated using the median values of all plots.

Please note that in the Dutch registration procedure, the target variable is the median concentration in time and the 90th percentile in space. This is different from the FOCUS procedure, where the 80th percentile in time is combined with an approximate 80th percentile in space.

2.14 Viewing maps and graphs

By clicking the Graphs and Maps button, the user has fast access to all spatially distributed model inputs and model outputs. This option is extremely powerful when analysing the behaviour of the model behaviour. Three major groups of variables can be accessed:

1. Spatially distributed model input parameters, which fall apart into two categories, i.e. soil parameters and crop areas. These parameters can be accessed through the 'Echo of Input' tab. As mentioned in Section 2.9, crop areas are used as a proxy for the area of usage.
2. Output parameters that are available for the total area of use; i.e. for the area of all crops included in the assessment.
3. Output parameters that are available for assessment items, i.e. for specific combinations of crops and application schemes included in an assessment.

It is always possible to review the model inputs, the other two tabs are only visible if an assessment has run successfully.

Some of the maps are prepared automatically after finishing the calculations. It will take only a few moments to present these maps on the screen. Other maps are prepared only upon request of the user. The preparation of these maps, i.e. the selection of appropriate results, may take several minutes.

Viewing input parameters

Maps of input parameters and maps of crop areas are available in the 'Echo of Input' tab (Figure 16). For viewing input parameters, check 'Map – Soil properties' and select the appropriate parameter from the drop-down box and the depth for which you want the parameter to be visualized. To view the crop areas, check 'Map – Crop area' and select the crop from the drop-down box.

Viewing output parameters for the total area of use

If you want to graph results for the total area of usage, select the 'Area of usage' tab (Figure 17). This tab is only visible if results are available. You can choose between two graphs:

- The first graph shows the cumulative frequency distribution of the median leaching concentration of each plot.
- The second graph shows the cumulative frequency distribution of the 20th, 50th and 80th percentiles of each plot. This graph is an extension of the first graph; it shows the variability of the leaching concentration due to variability in weather conditions.

Both graphs can be shown for all substances in an assessment; i.e. the parent and, if applicable, the metabolites.

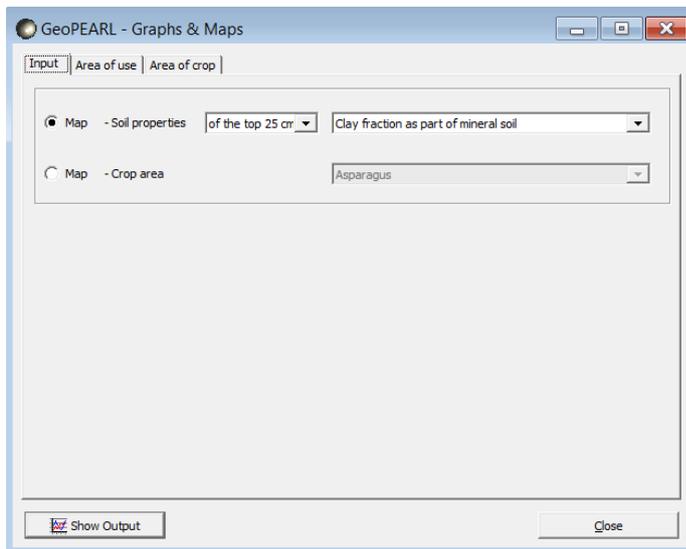


Figure 16 Screen for reviewing the input parameters.

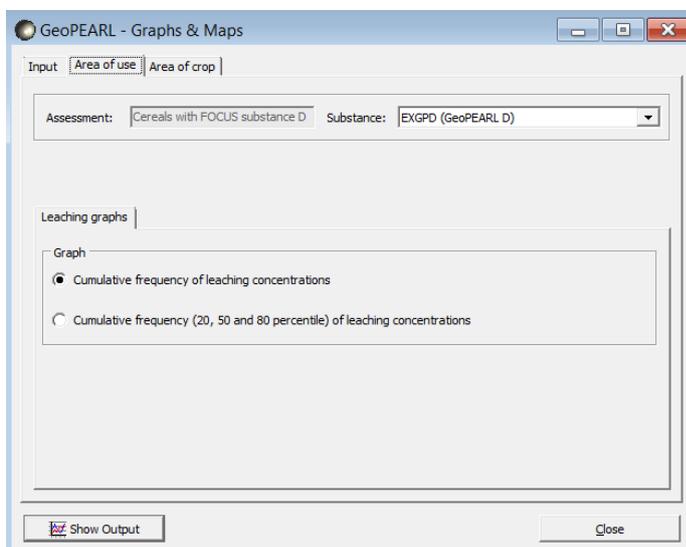


Figure 17 Screen for viewing output for the area of use of the substance in an assessment.

Viewing output parameters for individual crops within an assessment

If you want to graph results for the total area of usage, select the 'Area of crop' tab (Figure 18). This tab is only visible if results are available. First select the substance for which you want to view the output. You can choose between the following type of graphs:

- Cumulative frequency distribution of the median leaching concentration. In contrast to the graph in previous section, this graph pertains to a single crop only.
- Cumulative frequency distribution of the 20th, 50th and 80th percentile in time of the leaching concentration.
- Maps of the leaching concentration.
- Maps of terms of the water balance. A schematic overview of the water balance is presented in Figure 22.
- Maps of terms of the substance balance. A schematic overview of the substance balance is presented in Figure 23.

All maps are presented with five classes, all classes have the same area (automatic legend scaling). In the case of the leaching concentration, it is also possible to create a map with pre-defined classes. The advantage of a map with predefined classes is that the trigger concentration of $0.1 \mu\text{g L}^{-1}$ is clearly visible.

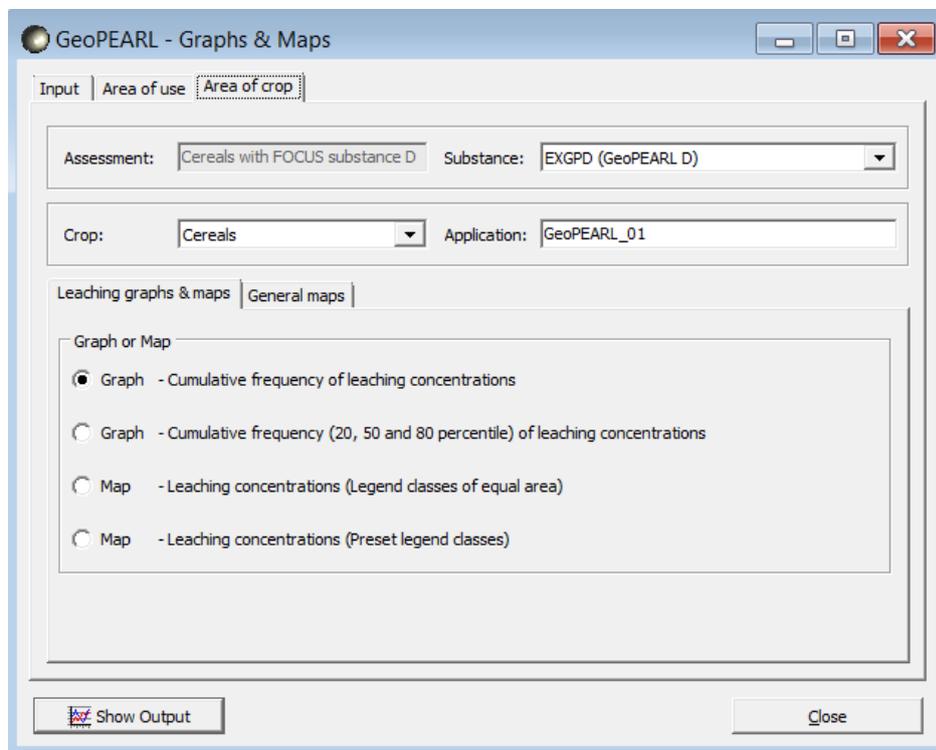


Figure 18 Screen for viewing output for individual crops within an assessment.

The viewer

GeoPEARL uses the graphical program XYWIN for all graphs and maps. Functions that are available within XYWIN are:

- Zooming: click the left mouse button to select a rectangle.
- *Warning: this function is only intended to analyse the map; it should not be used to 'read' the leaching concentration in your 'backyard'.*
- Statistics: you can use XYWIN to create frequency diagrams of maps.
- *Warning: if used for maps of the leaching concentration, this function may give different results than the cumulative frequency distribution generated by GeoPEARL itself. The reason is that blanks are treated in another way.*
- Printing: Graphs can be printed by pressing CNTRL-P or by selecting print from the file menu.

- Export of graphics files: Use the File menu select Output. You can specify different output formats, like jpg, png, tiff and emf. If you want to incorporate a graph in a word processor like Word, we advise to use png format.

2.15 Archiving your assessment

The GeoPEARL User Interface has the possibility to export the information that is required to run the assessment to ASCII files. The structure of these files is described in Chapter 3. This functionality can be accessed by selected Archive from the Assessment submenu at the main screen (or press Alt-A-A). The obtained files can be used:

- to archive your run;
- as input for the stand-alone version of GeoPEARL.

Please notice that it is currently not possible to import the obtained files into another GeoPEARL database. You must also archive the GeoPEARL database.

2.16 Directory structure for the GeoPEARL User Interface

The communication between the GeoPEARL User Interface and the GeoPEARL executables is through ASCII files. These files can also be used in combination with the stand-alone version of GeoPEARL, as described in Chapter 3.

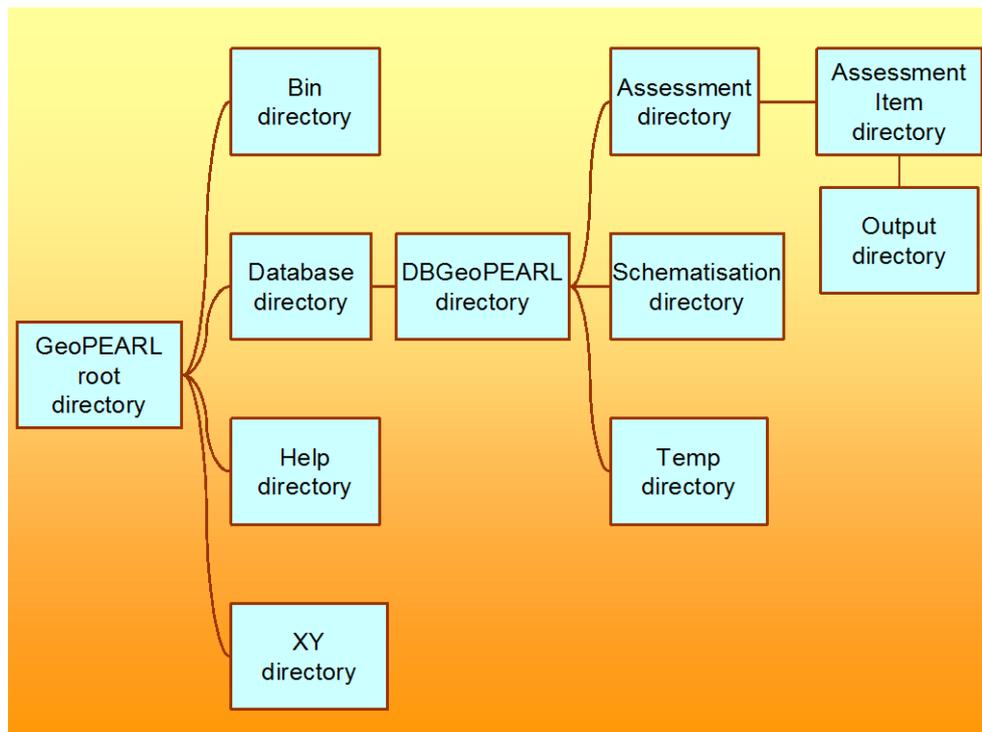


Figure 19 Directory structure for the GeoPEARL User Interface.

Figure 19 shows the directory structure used by the GeoPEARL User Interface:

- The GeoPEARL root directory is the directory that you have specified during the installation.
- The bin directory contains all executables.
- The database directory contains the GeoPEARL database. The default name of the database is dbGeoPearl.fdb.
- All ASCII files required by the GeoPEARL executable are stored in the dbGeoPEARL directory. The actual name of this directory depends on the name of the database. If, for example, the name of the database is assessmentsdossier1.fdb, the name of this directory would also have the name

'assessmentsdossier1'. The number of data directories is equal to the number of GeoPEARL databases.

- The next level is the Assessment directory. For each assessment that has been carried out with GeoPEARL, a directory is created. Directories are given numbers; the numbers correspond with the assessment number.
- Parallel to the Assessment directory, you will find the Schematisation directory. This directory contains all the ASCII files of the spatial schematisation (represented by a pink colour in Figure 20) and the output control file (ctr file).
- The Temp directory contains temporary files generated by the GeoPEARL executable.
- Within the assessment directory, you will find one or more assessment item directories. In this directory, you will find back the geo, cmp and app files (see Section 3.2 for explanation).
- The output of an assessment item is written to the output subdirectory (the files with a blue colour in Figure 20).

2.17 Using another GeoPEARL 4.4.4 database

You can use multiple database with GeoPEARL. To do so, follow this procedure:

- Go to the database directory and copy the database (i.e. the file with extension .fdb). The name of this database should be different from the name of the original database.
- From the main menu, select File – and then 'Open GeoPEARL database' to open another database;
- GeoPEARL will now open the other database.
- When starting GeoPEARL, it will open the database that was in use the last time the GeoPEARL application was running.

3 User's guide of the command-line version of GeoPEARL

This chapter describes the command-line version. Instructions are given how the model can be applied to applications in which the user primarily wants to change the substance properties and the application schedule. You will see that the steps for running the stand-alone version of GeoPEARL are almost the same as the steps to be followed when using the GeoPEARL User Interface. This manual is dedicated to the Dutch application. If you want to use GeoPEARL for other countries or areas, you have to create a new spatial schematisation first. Once done, the steps are exactly the same as in the Dutch application. Substance properties must be specified in the file with extension cmp (step 4 of 'Getting Started', see Section 2.5).

3.1 Performing an assessment with the stand-alone version

1. Download the 'geopearl_4_4_4_ascii.zip' archive from the PEARL website to get the schematisation files and model kernels as well as an example set of input files for the stand-alone version of GeoPEARL.
2. Copy the contents of the Example directory to a new directory. Assign a unique directory to each assessment. You can, alternatively, copy assessments from the GeoPEARL User Interface (see Section 2.17 for directory structure). Files generated by the GUI do, however, not have comment lines and are more difficult to understand.
3. Add a new substance to the compounds file and edit the substance properties (see manual SPIN v3.3 – Van Kraalingen *et al.*, 2019; i.v.).
4. Add a new application schedule to the applications file and edit it (Section 3.5).
5. Edit the geo file.
 - a. Specify the directory structure (Section 3.6.1).
 - b. Specify the control options of GeoPEARL (Section 3.6.2).
 - c. Specify the required spatial resolution and the crop for which a registration is requested (i.e. plot selection; Section 3.6.3).
 - d. Specify the substance and application schedule (Section 3.6.4 and 3.6.5).
 - e. Request additional (detailed) output (optional, Section 3.6.6).
6. Run the model (Section 3.7).
7. GeoPEARL creates a number of output files, containing the substance and water balances and percentiles of the leaching concentration (Section 3.8).
8. Use the 'percentiles.exe' executable to calculate the 90th percentile of the leaching concentration and generate maps.
9. The tables can be imported in EXCEL for additional calculation or in a Geographic Information System to generate maps and regional scale substance and water balances (Section 3.10)

3.2 File structure

Figure 20 gives an overview of all files types. Each file type has its own extension, the extension may not be changed. There are three groups of files:

- Files that need to be edited in standard applications. These files are given a green colour in Figure 20 and are stored in the example directory.
- Files that contain the spatially distributed parameters. These files should not be changed, unless a new spatial schematisation is set-up by the user. These files are given a pink colour in Figure 20 and stored in the schematisation directory.
- Output files (blue colour), which are stored in the output directory.

The position of all files can be changed (see further Section 3.6). This report describes the green and blue files only, as these are the files that are relevant for standard applications. A description of the other files can be found at the PEARL website (<http://www.pearl.pesticidemodels.eu>).

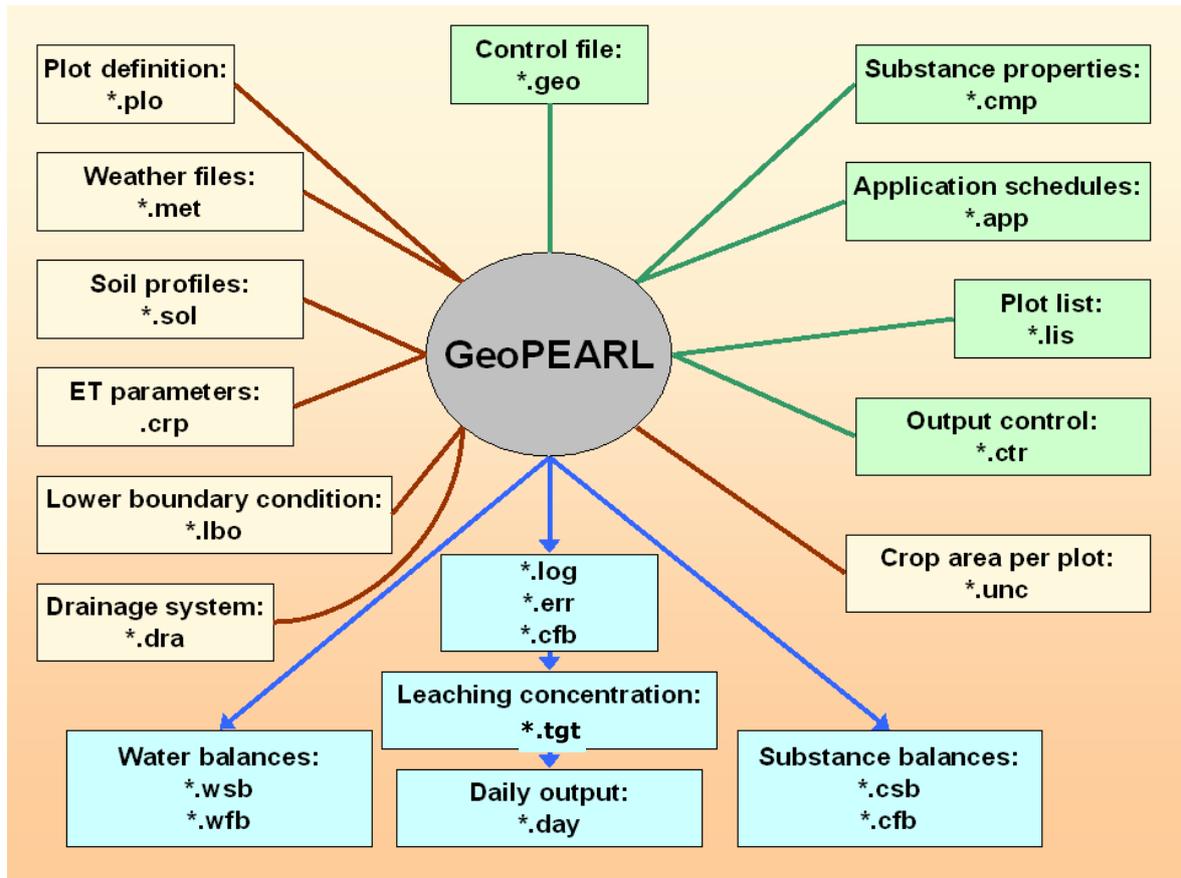


Figure 20 File structure of GeoPEARL. Files with a green colour are stored in the assessment directory, files with a pink colour in the schematisation directory. Only files with a green colour need editing.

3.3 Creating an assessment with multiple assessment items

As described in Section 2.2, a GeoPEARL assessment is carried out for a single substance, but may consist of several so-called assessment items. Assessment items are combinations of a crop for which a registration is asked and an application scheme. This implies that different crops can have different application schemes. To carry out an assessment with more items, do the following:

1. After having created the geo file for the first crop, copy this file as many times as there are items in your assessment. If, for example, you have to do an assessment for maize, potatoes and cereals, create a file maize.geo, potatoes.geo and cereals.geo
2. In each geo file, assign the appropriate crop in the Crops table and the appropriate application schedule in the applications table. Warning: these two variables are the only variables that can be different within an assessment! You can only use one substance within an assessment.
3. Run the model for all items.
4. Use the percentiles.exe program to:
 - a. calculate the overall 90th percentile of the leaching concentrations at the total area of usage;
 - b. calculate the 90th percentile of the leaching concentrations for each assessment item individually;
 - c. generate maps.

The percentiles program should be run one time in an assessment. The entire procedure is described in Figure 21.

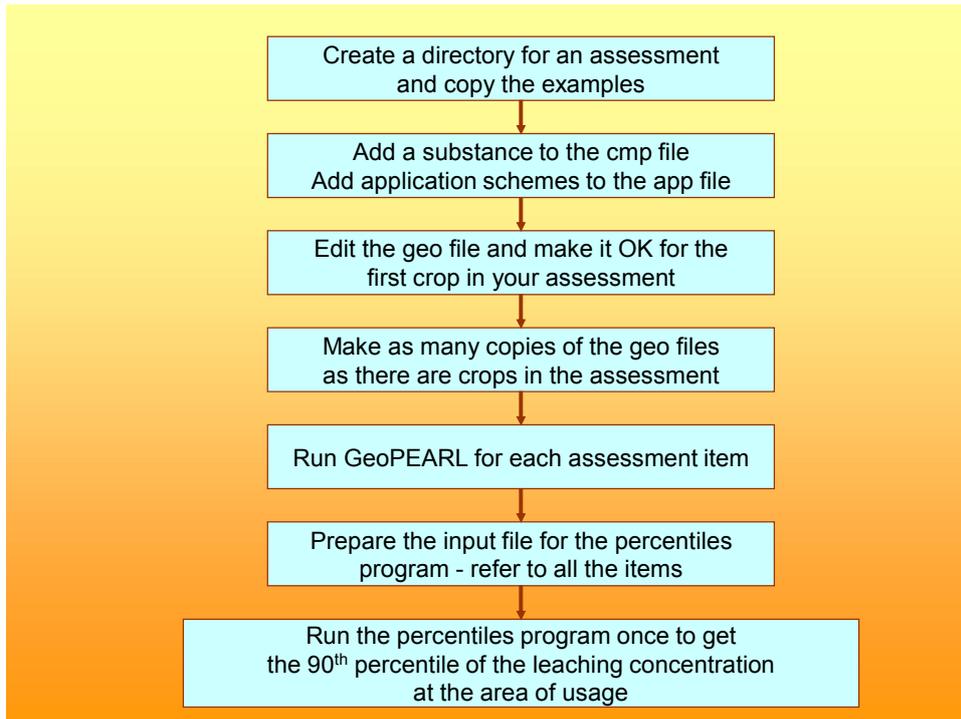


Figure 21 Performing an assessment with multiple assessment items with the stand-alone version of GeoPEARL.

3.4 Adding and editing application schemes

Application schemes must be specified in the file with extension app (step 5 in Section 2.5 'Getting Started'). An example of this file is included in the examples directory. We recommend to make a copy of this file before editing.

Each application scheme starts with [scheme] and ends with [end_scheme], where scheme must be replaced by the actual name of the application scheme. Each section contains the following parameters:

- DelTimEvt: The application interval in years. Its value can be set to 1, 2 or 3. If set to 2, for example, biennial applications are simulated. Conform the FOCUS procedure (FOCUS, 2008), the simulation length (26, 46 or 66 years) is dependent on the value of this parameter.
- Table Applications: The applications table. The first columns contains the application date, the second column the application type, the third column the dosage and the fourth column the injection or tillage depth (if relevant).

```
*-----*
*
* Application schemes
*
* Column 1: Date
* Column 2: Application type: AppSolSur, AppSolInj, AppSolTil, AppCrpUsr
*
* If Type = AppSolSur (soil surface application):
* Column 3: Dosage (kg/ha) [0|-]
*
* If Type = AppSolInj (injection):
* Column 3: Dosage (kg/ha) [0|-]
* Column 4: Injection depth (m) [0|-]
*
* If Type = AppSolTil (tillage):
* Column 3: Dosage (kg/ha) [0|-]
* Column 4: Tillage depth (m) [0|-]
*
```

```

* If Type = AppCrpUsr (application to the crop canopy):
* Column 3: Dosage (kg/ha) [0|-]
* Column 4: Fraction of dosage applied to the crop canopy (-) [0|1]
*
*-----
*-----
* Application to the soil surface in spring

[springsurface]

1      DelTimEvt      Application interval

table Applications
26-May AppSolSur 1
end_table

[end_springsurface]

```

3.5 Editing the main .geo file

All other changes for standard runs must be made in the geo file. An example of this file is in the root directory of GeoPEARL (i.e. the directory where GeoPEARL was installed). Make sure to make a copy before editing this file. An example of the new geo file is presented in Annex 2.

3.5.1 Specifying the input- and output directories

The directory where files are read or put can be changed. The position of files containing the spatial schematisation must be specified in the SchematisationDir record, the position of the output files in the OutputDir record and temporary files are stored in the PearlDir. Warning: if files are stored in a directory with spaces in its name, use relative paths only – otherwise GeoPEARL will not find these files.

```

* Directory structure
* The input directory is obtained from the model call.
..\Schematisation  SchematisationDir  Spatial schematisation
Output            OutputDir          Output directory
Tmp               PearlDir           Tmp directory for PEARL runs

```

The following files can be put at any place:

- PlotListFile: file with plots to be simulated.
- CompoundProperties: file with substance properties.
- ApplicationSchemes: file with application schemes.
- OutputControl: output control file.

Therefore, the full path of these four files should be given at any time. The path name can, however, be relative to the position of the geo file (for example ..\examples\example.cmp).

3.5.2 Controlling the simulations

GeoPEARL has various options to control the simulation (step 6b of 'Getting Started').

- IOMode: Screen control. If set to 'IOMode_StdOut', screen output is limited and can be redirected to 'stdout', if wanted. If set to 'IOMode_Full', screen output is complete, but results cannot be captured to a text file.
- PriorityClass: Priority class for PEARL call. Can be set to Low, Normal or High. If GeoPEARL runs on a computer where you want run GeoPEARL in background, set PriorityClass to Low, otherwise choose a different option.
- OptAppend: OptAppend can have four values, i.e. 'Yes', 'No', 'SkipErrors' and 'New'
 - If set to 'Yes', results are appended to existing output files. If a plot has previously resulted in an error, a retry will be carried out.
 - If set to 'SkipErrors', results are appended to existing output files and plots that have previously resulted in an error will be ignored.

- If set to 'No', new files will be created. Existing files with the same name will be replaced without further notice.
- If set to 'New', new files will be created. If files exist already with the same name, GeoPEARL will give an error message.
- OptDelPloFiles: If set to 'Yes', GeoPEARL removes all temporary files when a plot is done (see the flow diagram in figure 11 of GeoPEARL report, Tiktak *et al.*, 2013). This option should not be changed, unless you are testing the model.
- OptHyd: GeoPEARL can be used to simulate water balances only. Set OptHyd to Only to do so. See also Section A1.6 of the FOCUS PEARL user manual.
- TimStart: The start-time of the simulations. For the Dutch registration procedure, Tim-Start should be 01-Jan-1901.
- TimEnd: The end-time of the simulations is dependent of the repeat interval of applications as specified in the applications file. It should be set to 31-Dec-1926 in the case of annual applications, 31-Dec-1946 in the case of biennial applications and 31-Dec-1966 in the case of triennial applications. See also Section A1.6 of the FOCUS PEARL user manual.
- IniYears: The number of initialization years. These years or not used for the calculation of the percentiles of the annual leaching concentration. The value to be used in the registration procedure is 6.
- NumCPU: Maximum number of CPUs available. If GeoPEARL is used in a classical configuration, put NumCPU to 1. For further explanation of the grid-option, refer to Section 3.11.
- CPUID: The CPU ID. If GeoPEARL is used in a classical configuration with one CPU only, put CPUID to 1.

```

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

IOMode_StdOut  IOMode           Screen control [IOMode_Full|IOMode_StdOut]
Normal        PriorityClass     Priority class [Low|Normal|High]
Yes           OptAppend       Should files be appended?
Yes           OptDelPloFiles   Should the other plot files be removed?
Automatic     OptHyd           SWAP mode: Automatic|OnLine|Only
01-Jan-1901   TimStart        Start time of the simulation
31-Dec-1926   TimEnd          End time of simulation
6             InitYears       Number of years for initialization
1             NumCPU         Number of CPUs for grid computing (1|-)
1             CPUID        Number of the current CPU (1|NumCPU)

```

3.5.3 Plot selection

GeoPEARL has two options to select the plots to be included in the simulations, i.e. manually or automatically on the basis of the area of potential pesticide usage (i.e. area of the crop in which the substance is applied; see Section 2.5 of Tiktak *et al.* (2003). In the second case, plots are aggregated to larger computational units referred to as 'zones'. Selection between the two options of plot selection is done by setting the variable OptPlotList. The default in registration is 'Automatic'. If the user chooses for automatic plot selection, the results of the plot selection are written to a file extension with crf.

- OptPlotList has three options, i.e. 'Automatic', 'Manual' and 'Generate_Only':
 - If OptPlotList is set to 'Manual', the user must supply a file with plot numbers that must be included in the simulation. The name of this file (with extension .lis) should be specified in the record PlotListFile. Manual plot selection is particularly handy for testing as it makes it possible to run a single plot and check if the model runs well.
 - If OptPlotList is set to 'Automatic', the user must specify the crops for which a registration is requested (table Crops). You can chose between one of the crops included in table 2 of the GeoPEARL report. The user must specify three additional parameters, i.e. NumZone, ThresholdArea and OptPlotSelection.
 - If OptPlotList is set to 'Generate_Only', GeoPEARL will create a list with plot numbers to be included in the simulations, without actually starting the simulations. Results are written to a file with extension crf.
- CropAreaDataBase: The name of the file with information on crop areas per plot. The extension of this file is unc.

- NumZone: The number of zones. Although the minimum number of zones is 10, at least 250 zones should be used for reliable results. Choosing a lower resolution should only be done when performing a quick-scan; runs with a low resolution are not accepted for the final registration.
- ThresholdArea: Plots with a crop area below this threshold are not included in the simulations. The default setting is 0.01 ha.
- OptPlotSelection: Method for allocation of plots to zones. If option 'Rank' is chosen, plots are aggregated on the basis of their relative vulnerability index. If option 'Neighbour' is selected, adjoining plots are put together. Option 'Rank' performs best for ordinary substances, otherwise the 'Neighbour' option should preferably be selected.

```

*-----
* Reference to plot file and plots included in model run
*-----
holland      Plots          Plot file (plo file, must be in plot directory)
Automatic    OptPlotList      Plot list: [Automatic|Manual|Generate_Only]

*-----
* If OptPlotList = Manual:
example      PlotListFile     File with plots to be simulated

*-----
* If OptPlotList = Automatic:
holland      CropAreaDatabase  Files with crop area per UC (unc file)
0.01         ThresholdArea    (ha)    Threshold area (0|-)
250         NumZone         Number of zones (100|NumPlo)
Rank        OptPlotSelection Option for plot selection [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
1 Potatoes
end_table

```

GeoPEARL version 4.4.4 has also an option to select plots on the basis of a range of values for the soil property selected by the user. More information on this option is given in Van den Berg *et al.* (2008).

3.5.4 Specification of compounds and applications to be included in the simulation

The final stage of editing consists of specifying the compounds and applications schemes that should be included in the simulations. There are three parameters that need to be edited:

- CompoundProperties: Full name (including directory name) of the file with substances properties. This file must have extension cmp. An example can be found in the examples directory.
- ApplicationSchemes: Full name of the file with application schemes. This file must have extension app. An example can be found in the examples directory.
- Table Runs: The first column of this table contains the substance name and the second column contains the application scheme to be included in the simulation. The following columns contain the code for each individual parent or daughter compound. Be sure that all names and codes match names and codes in the substances and applications files, respectively.

```

*-----
* Compound and application information
*-----
example      CompoundProperties  File with compound properties
example      ApplicationSchemes  File with 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
NLA springsurface NLA1 NLA2
end_table

```

3.5.5 Specification of the ploughing parameters

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 type: 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 Annex 1.

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

* tableCtgb_Crops
* 1 Potatoes
* 2 Strawberries
* 3 Asparagus
.
.
* 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
.
.
end_table
```

3.5.6 Specification of the spatial schematisation

The following sections of the geo file contains references to the files with spatially distributed parameters. In standard applications, these sections do not need editing. References must be made to the soils file (SoilDatabase), the file with crop related evapotranspiration data (CropDatabase), the weather files (MeteoStations), the file with data on the lower boundary condition of SWAP (GroundwaterSystem) and the file with parameters of the local drainage system (DrainageSystem). The position of all these files must be specified in the SchematisationDir (see Section 3.5.1).

```
*-----
* Soil information (files must be stored in soil directory)

holland      SoilDatabase      Soil database

*-----
* Crop information (file must be stored in crops directory)

holland      CropDatabase      File with crop properties (extension crp)

*-----
* Information about meteo stations
* 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

table MeteoStations
1      52.0    10.0    9.97    Input    DeKooy
2      52.0    10.0    9.97    Input    Leeuwarden
3      52.0    10.0    9.97    Input    Eelde
4      52.0    10.0    9.97    Input    Hoorn
5      52.0    10.0    9.97    Input    Lelystad
```

6	52.0	10.0	9.97	Input	Dedemsvaart
7	52.0	10.0	9.97	Input	Naaldwijk
8	52.0	10.0	9.97	Input	DeBilt
9	52.0	10.0	9.97	Input	Winterswijk
10	52.0	10.0	9.97	Input	Andel
11	52.0	10.0	9.97	Input	Vlissingen
12	52.0	10.0	9.97	Input	Oudenbosch
13	52.0	10.0	9.97	Input	Gemert
14	52.0	10.0	9.97	Input	Venlo
15	52.0	10.0	9.97	Input	Beek

end_table

```

*-----
* Local and regional groundwater system
holland      GroundwaterSystem      Groundwater system (lbo file)
holland      DrainageSystem            Local drainage system (dra file)

```

3.5.7 Output and SWAP control

All other parameters of the geo file can be left at default values.

```

*-----
* Output control data

Yes          OptScreen                Screen option (No|Swap_Only|Yes)
Schematisation OutputControl            File with output data (ctr file)
Yes          PrintCumulatives         Print fluxes cumulative (Yes|No)
Fixed       OptZTgt                  Option for OptZTgt (Fixed|Variable)
1           ZTgt                    (m) Depth of layer for balances (0.1|-)
0.05       ThiLayEAD              (m) Ecotoxicological Averaging Depth (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
No         OptPersistency         Calculate persistency (Yes or No)

*-----
* SWAP control parameters

No          OptHysteresis           Simulate hysteresis (No|Yes)
100         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)

```

The option OptPersistency can be selected to assess the persistence of compounds in the top layer of the soil (as specified by ThiLayEAD) at two or seven years after the last application.

3.6 Running the model

Once all files have been edited, the model can be run. The command call consists of two parts; i.e. *the program name and the name of the run*. The name of the run is exactly the same as the name of the control file (the geo file). The full name *including the directory name* should be specified here. The command can also be given from a command box or from Windows Explorer. After you have entered this command, the program will start. A flowchart, which gives the order of the calculations, is given in Figure 11 of the GeoPEARL manual. If you have set the option PriorityClass to Low, the program will run in background – you can then continue working on other projects without problems. During program execution, you should not logoff. The program can be aborted any time by entering CNTRL-Break. If you have set OptAppend to Yes, you can restart where you ended.

3.7 Output files

3.7.1 General

GeoPEARL writes its results to a total number of nine output files, which are all stored in the output directory. The following file extensions are generated (see also Figure 20):

- **wsb**. These files contain the annual and long-term average water balances of the soil profile.
- **wfb**. These files contain the annual and long-term average water balances of the FOCUS layer. The thickness of the layer is set by the variable ZTgt in the output control section of the geo file. Following recommendations of the FOCUS working group (FOCUS, 2000), its default value is 1 m.
- **csb**. These files contain the annual and long-term average substance balances of the soil profile.
- **cfb**. These files contain the annual and long-term average substance balances of the FOCUS layer. The thickness of the layer is set by the variable ZTgt in the output control section of the geo file. Following recommendations of the FOCUS working group (FOCUS, 2000), its default value is 1 m.
- **ccb**. These files contain the annual and long-term average substances balances of the crop canopy.
- **tgt**. These files contain the percentiles of the leaching concentration at target depth. The target depth is set by the variable ZTgt in the output control section of the geo file. Following recommendations of the FOCUS working group (FOCUS, 2000), its default value is 1 m.
- **day**. If detailed (daily) output is requested in the control file, results are written to these files. In standard applications, these files are empty.
- **log**. This file contains the program log. You can review, for example, the computation times and see which plots have been done so far.
- **err**. Error messages are written to these files.
- **crf**. This file is generated if you have set OptPlotList to Automatic (Section 3.6.3). This file gives the linkage between the zone numbers and the plot numbers and is needed when creating output maps.

3.7.2 The water balance of the individual plots (wsb and wfb files)

GeoPEARL gives, for each plot, the following annual and long-term average terms of the water balance (see also Figure 22; the numbers refer to the column numbers in the files):

1	Plot	The plot number	
2	Yr	The year or 'Avg' for long-term averages	
3	Delliq	Net storage change of water in profile	(m.a-1)
4	Prc	Precipitation	(m.a-1)
5	Irr	Irrigation	(m.a-1)
6	FlvLea	Seepage at the lower boundary	(m.a-1)
7	FlvGrw	Groundwater recharge	(m.a-1)
8	EvpInt	Evaporation of intercepted water	(m.a-1)
9	SolAct	Actual soil evaporation	(m.a-1)
10	TrpAct	Actual transpiration	(m.a-1)
11	Dra	Total discharge to drains and channels	(m.a-1)
12	Dra_1	Lateral discharge to primary system	(m.a-1)
13	Dra_2	Lateral discharge to secondary system	(m.a-1)
14	Dra_3	Lateral discharge to tertiary system	(m.a-1)
15	Dra_4	Lateral discharge to tube drains	(m.a-1)
16	Dra_5	Lateral discharge to surface drainage system	(m.a-1)
17	Run	Run-off	(m.a-1)
18	EvpPnd	Evaporation of ponded water	(m.a-1)
19	SolPot	Potential soil evaporation	(m.a-1)
20	TrpPot	Potential transpiration	(m.a-1)

The water balance is as follows and can be checked by importing the **wsb** and **wfb** files in a spreadsheet (for example EXCEL):

$$Delliq = Pr c + Irr - EvpInt - Run - SolAct - TrpAct - Dra - FlvLea \quad (1)$$

where *Delliq* is the storage change. Please notify that the lower boundary flux, *FlvLea*, is negative if downwards. The groundwater recharge is calculated by integrating the flux over the phreatic groundwater table. In those cases where there is no local drainage system, this flux should be equal to the lower boundary flux (*FlvLea*).

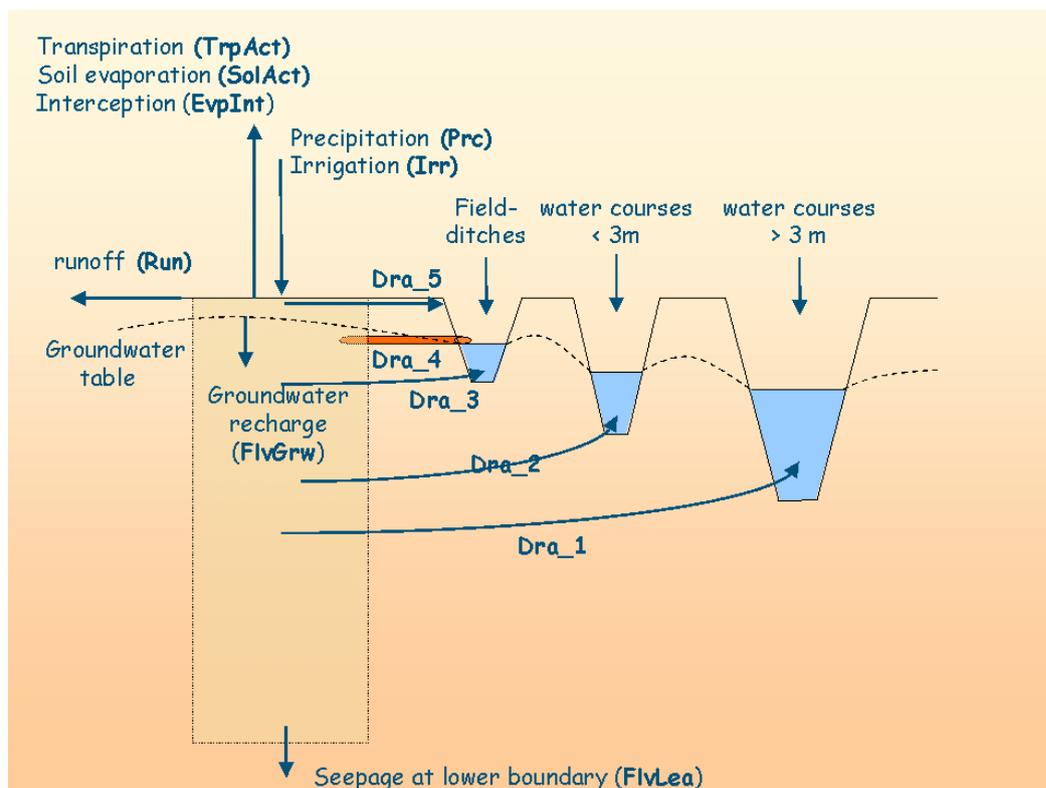


Figure 22 The GeoPEARL water balance.

3.7.3 The substance balance of the individual plots (csb and cfb files)

Terms of the substance balance are given for all compounds (i.e. for both parents and metabolites). The **cfb** and **csb** contain the following columns (see also Figure 23):

1	Plot	The plot number	
2	Substance	Name of substance	
3	Application	Name of application scheme	
4	Yr	The year or 'Avg' for long-term averages	
5	Cmp	Compound code	
6	AmaAppSol	Areic mass applied to the soil system	(kg.ha-1.a-1)
7	DelAma	Change of mass in the soil system	(kg.ha-1.a-1)
8	DelAmaEq1	Change of mass in the equilibrium domain	(kg.ha-1.a-1)
9	DelAmaNeq	Change of mass in the non-equilibrium domain	(kg.ha-1.a-1)
10	AmaTra	Areic mass transformed in the soil system	(kg.ha-1.a-1)
11	AmaFor	Areic mass formed in the soil system	(kg.ha-1.a-1)
12	AmaUpt	Areic mass taken-up from the soil system	(kg.ha-1.a-1)
13	AmaDra	Areic mass drained from the soil system	(kg.ha-1.a-1)
14	AmaDra_1	Areic mass drained to the primary system	(kg.ha-1.a-1)
15	AmaDra_2	Areic mass drained to the secondary system	(kg.ha-1.a-1)
16	AmaDra_3	Areic mass drained to the tertiary system	(kg.ha-1.a-1)
17	AmaDra_4	Areic mass drained to tube drains	(kg.ha-1.a-1)
18	AmaDra_5	Areic mass drained to surface drain system	(kg.ha-1.a-1)
19	AmaDep	Areic mass deposited at the soil surface	(kg.ha-1.a-1)
20	AmaVol	Areic mass volatised from the soil surface	(kg.ha-1.a-1)
21	AmaLea	Areic mass leached from the soil system	(kg.ha-1.a-1)
22	AmaGrw	Areic mass leached into the deep aquifer	(kg.ha-1.a-1)

The substance balance is as follows and can be checked by importing the csb and cfb files in a spreadsheet (for example EXCEL):

$$DelAma = AmaApp + AmaDep - AmaVol - AmaLea - AmaUpt - AmaDra - AmaTra + AmaFor \quad (2)$$

where *DelAma* is the areic mass balance change. As with the water balances, net downward fluxes are negative.

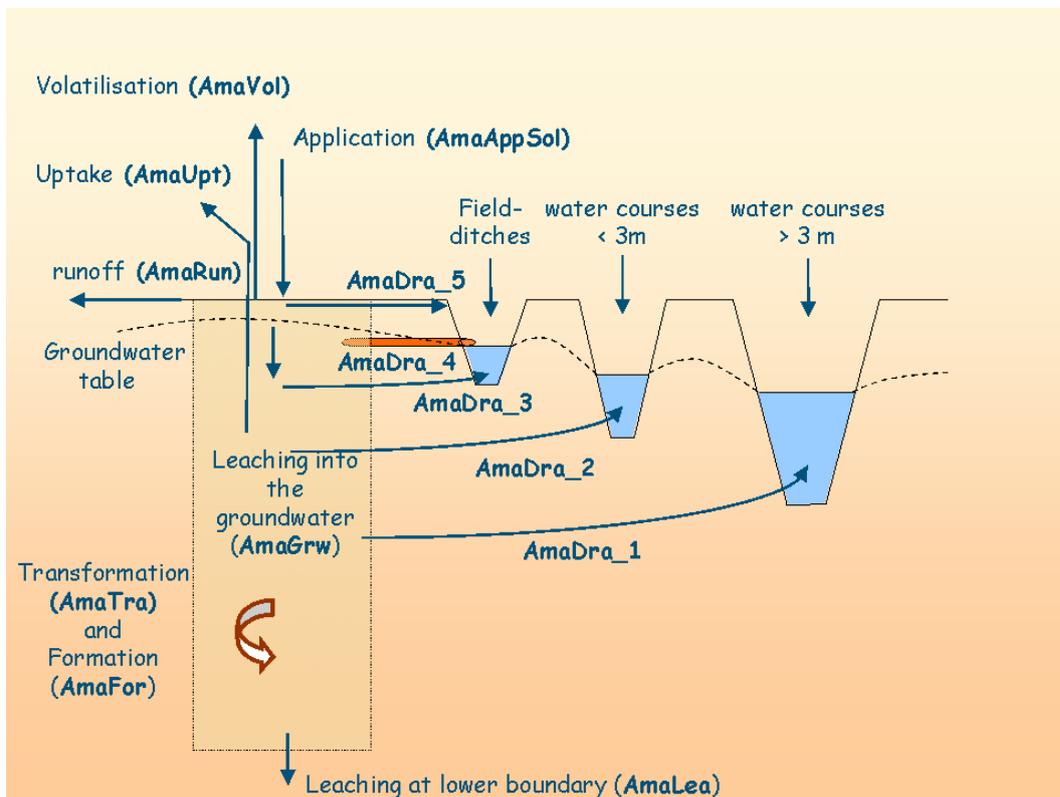


Figure 23 The GeoPEARL substance balance.

3.7.4 Percentiles of the leaching concentration (tgt file)

Percentiles in time of the mean annual leaching concentration at target depth are output to the file with extension **tgt**. The default value for the target depth is 1 m and can be controlled by the variable ZTgt in the output control section of the geo file (Section 3.5.6). For standard applications it should, however, not be changed. The calculation procedure for the percentiles is essentially the same as in the FOCUS procedure (FOCUS, 2000).

To have correct percentiles generated, the simulation must conform to FOCUS requirements, which implies that:

- Repeated applications should be simulated by setting DelTimEvt in the control file to 1, 2 or 3 (Section 3.4)
- The simulation length must be 26, 46 or 66 years, depending on the value of DelTimEvt. The simulation length is controlled by the variable TimEnd, which should be set to 31 Dec 1926, 31-Dec-1946 or 31-Dec-1966.
- The initialization period must be six years. The length of the initialization period is controlled by the variable InitYears (Section 3.4.3).

The tgt files contain the following columns:

1 Plot	The plot number	
2 Substance	Name of substance	
3 Application	Name of application scheme	
4 Cmp	Compound code	
5 Perc	Percentile with respect to weather conditions	
6 Year	The year	
7 ConLea	Leaching concentration at target depth	(ug.L-1)

In contrast to the European registration procedure, where 80th percentile of the leaching concentration is selected, *the target percentile for the Dutch registration procedure is the 50th percentile (i.e. the median value).*

Link between zones and plots (crf file)

As specified before, GeoPEARL can aggregate plots to larger computational units called zones. Within each zone, the largest plot ('dominant plot') is assumed representative for the entire zone. Calculations are carried out for the dominant plot only. When making graphs or regional scale substance and water balances, the user needs a link between the zone number and the plot number. This link is given in the plot table of the crf file. The format of this file table is as follows:

1 Plot	The plot number
2 Zone	The zone number
3 Area	Area of plot
4 AreaCrop	Area of crop for which a registration is requested in plot
5 RelArea	Relative area of crop per plot (%)

3.7.5 Other output files

There are three additional output files:

- The **day** file, which contains detailed output. This file is only generated if additional output was requested by the user (Section 3.5.6). The format of the day file is exactly the same as the format of the output file of FOCUS PEARL, so it is not further discussed here.
- The **log** file, which contains log information such as the computation time per plot.
- The **err** file, which contains error messages. If the model terminates normally, it should be empty.

3.8 The percentiles program

Summary reports, including the 90th percentile of the leaching concentration at the area of usage are generated by the percentiles program. To use this program, the following steps must be followed:

1. Create an assessment file. This file must have the extension .ass.
2. Edit this file. It is important to make a reference to all assessment items to get the appropriate 90th percentile.
3. Run the program percentiles.exe.
4. Results are written to a file with extension .per.

3.8.1 The assessment file

An example assessment file is listed below. An example is included in the example directory as well.

```
*-----  
*  
* Input file for the calculation of percentiles and maps of an assessment  
* --> Initial version  
*  
1 ModelVersion  Model version  
1 GUIVersion   GUI version  
1 DBVersion    Database version  
*-----
```

Percentiles.exe has the possibility to create maps of the 90th percentile of the leaching concentration. To use this option, set OptShowMaps to Yes. Maps have an automatic or predefined legend. This is controlled by the OptAutoScaling variable.

```
* General control parameters  
No           OptAppend      Append results to existing output files  
Yes          OptScreen     Screen output?  
Yes          OptShowMaps   Show the maps?  
No           OptAutoScaling  Auto scaling in maps (Yes|No)?
```

In the following section, you have to specify the directory structure. Both absolute and relative paths are possible.

```
* Directory to which the output file is written
output                OutputDir                Output directory
..\schematisation    SchematisationDir    Schematisation
..\bin                XYDir                XY Directory
```

The next part refers to some basic maps. This section does not need editing.

```
* Map with unique combinations (must be in schematisation directory)
Holland_UC.map        UCMAP                Map with unique combinations
Holland.pol           Polygons             Map with country delineation
```

In this section, specify the assessment items that are part of the assessment. Please specify both the crop and the name of the file (including the path).

```
* Crops and files to be included in the assessment
* Both the crf and the tgt files must be present
table Assessment
1 maize output\maize
2 potatoes output\potatoes
3 cereals output\cereals
end_table
```

3.8.2 Running the program

Once the assessment file has been edited, the program can be run. The command call consists of two parts; i.e. *the program name and the name of the assessment*. The name of the assessment is exactly the same as the name of the control file (the ass file). The full name *including the directory name* should be specified here. The command can also be given from a command box or from Windows Explorer.

3.8.3 Output of the program

The program gives three different tables:

1. The leaching concentration for each zone included in the assessment. Zones are sorted on the basis of the leaching concentration.
2. Percentiles of the leaching concentration.
3. The final summary, including the 90th percentile of the leaching concentration and the total area.

Notice that the overall percentiles are calculated for all items included in the assessment. If you want to calculate percentiles for a single crop, you have to create an assessment file with one crop.

References

- FOCUS (2000). FOCUS groundwater scenarios in the EU review of active substances. Report of the FOCUS Groundwater Scenarios Workgroup, EC Document Reference Sanco/321/2000 rev.2, 202pp
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- Van den Berg, F., A. Tiktak, J.J.T.I. Boesten, A.M.A. van der Linden (2016). PEARL model for pesticide behaviour and emissions in soil-plant systems, 132 pp.
- Van den Berg, F., A. Tiktak, T. Hoogland, A. Poot, J.J.T.I. Boesten, A.M.A. van der Linden, J.W. Pol (2017). An improved soil organic matter map for GeoPEARL_NL. WENR report 2816, Wageningen Environmental Research, Wageningen, The Netherlands, 54 pp.
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Justification

This manual is an update of the manual for the use of GeoPEARL 2.2.2 and the addendum for the use of GeoPEARL version 3.3.3. The manual had to be updated, because a new version of GeoPEARL has been prepared, i.e. GeoPEARL v 4.4.4.

The project was supervised by Jennie van der Kolk (contact of WOT N&M, theme Agri-environment) and seen and approved by Miranda Meijsters (Ministry of Agriculture, Nature and Food Quality).

Annex 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
```

Annex 2 The GeoPEARL_4.4.4 input file – Expert users

This annex gives a listing of the GeoPEARL_4.4.4 input file. This file is intended to be used by expert users.

```
*-----
* GeoPEARL input file, generated by GeoPEARL 4.4.4
*
GEOPEARL CallingProgram
4.4.4 CallingProgramVersion
*-----

*-----
* 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
CMPEXGPD GeoPEARL_01 EXGPD
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   Oudembosch
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
*-----
* Output control data

Yes                               OptScreen                    Screen option (No|Swap_Only|Yes)
Schematisation                   OutputControl                File with output data (ctr file)
Yes                               PrintCumulatives             Print fluxes cumulative (Yes|No)
Fixed                             OptZTgt                      Option for OptZTgt (Fixed|Variable)

```

1	ZTgt	(m)	Depth of layer for balances (0.1 -)
0.05	ThiLayEAD	(m)	Ecotoxicological Averaging Depth (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
No	OptPersistency		Calculate persistency (Yes or No)

*-----

* SWAP control parameters

No	OptHysteresis		Simulate hysteresis (No Yes)
100	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)

*-----

* New parameters

Yes	OptDelOutFiles		Option to delete detailed output
None	OptAux		Option for auxiliary output
No	OptMacropore		Option for macropore flow
No	OptSnow		Option to consider snow in SWAP
No	OptNoResVert		Switch on or switch off vertical
resistance			
50	TargetPercentile (%)		Target percentile for leaching

* End of file

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