User manual for FOCUSPEARL version 5.5.5

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Abstract

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In the EU registration procedure, the assessment of the leaching to groundwater and the exposure of soil organisms as a result of the use of plant protection products is based on the use the FOCUS groundwater scenarios and the EFSA soil exposure scenarios, respectively. This user manual describes the use of the graphical user interface of the new FOCUSPEARL version, i.e. version 5.5.5, that facilitates the application of the scenarios for these assessments. In addition a description of the input and output files is given which helps the user to use the FOCUSPEARL model without the interface.

Keywords: crop protection product, FOCUS, PEC-Soil, groundwater, soil organisms, leaching, pesticide

Preface

This manual has been prepared to support the user of the new version of FOCUSPEARL, i.e. version 5.5.5. In this version, the EFSA soil exposure scenarios have been implemented in order to accommodate the assessment of the exposure of soil organisms.

The FOCUS groundwater scenarios have not changed in this version, except for a few corrections in the scenario data.

The FOCUSPEARL 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 FOCUSPEARL is coupled to SPIN version 3.3.

Contents

Summary

The FOCUSPEARL version 5.5.5 is presented in this report. PEARL is an acronym of Pesticide Emission Assessment at Regional and Local scales. This version supports the application of the FOCUS Groundwater scenarios and the EFSA Soil exposure scenarios.

The data for the groundwater scenarios are the same as those in FOCUSPEARL v.4.4.4, except that a few data were modified, because the data for these parameters in the database of the previous version were not correct. Other input data were adjusted to bring them in line with the parameterization of the soil exposure scenarios.

This report gives guidance on the use of the new FOCUSPEARL 5.5.5 version. The FOCUSPEARL software package consists of a set of computation kernels, a Graphical User Interface and a database with the scenario data for the FOCUS Groundwater scenarios and those for the EFSA Soil exposure scenarios.

The new version of the database of FOCUSPEARL does no longer contain the data on the physico-chemical properties of the compound. Instead, the new FOCUSPEARL version is coupled to the SPIN application to enter, edit or archive all substance data needed for a FOCUSPEARL run. The new version of FOCUSPEARL is coupled with FOCUSSPIN version 3.3

Samenvatting

Dit rapport introduceert FOCUSPEARL version 5.5.5. PEARL is een acroniem van Pesticide Emission Assessment at Regional and Local scales. Deze versie ondersteunt de toepassing van de FOCUS Grondwaterscenario's en de EFSA scenario's voor de blootstelling van bodemorganismen.

De gegevens voor de grondwaterscenario's zijn dezelfde als die in FOCUSPEARL v.4.4.4, behalve dat enkele gegevens zijn gewijzigd, aangezien de gegevens voor deze parameters in de vorige versie niet correct waren. Andere invoergegevens zijn gewijzigd om ze op een lijn te krijgen met de parameterisatie van de scenario's voor de blootstelling van bodemorganismen.

Dir rapport biedt ondersteuning voor het gebruik van de nieuwe FOCUSPEARL versie 5.5.5. Het FOCUSPEARL softwarepakket bestaat uit een set rekenmodellen, een gebruikersinterface en een database met de scenariogegevens voor de FOCUS Grondwaterscenario's en die voor de EFSA scenario's voor de blootstelling van bodemorganismen.

De nieuwe versie van de database van FOCUSPEARL bevat niet langer de gegevens over de fysisch-chemische eigenschappen van de stoffen. In plaats daarvan is de nieuwe versie van FOCUSPEARL gekoppeld aan de SPIN applicatie, waarmee de gegevens voor de stoffen die nodig zijn voor een FOCUSPEARL run ingevoerd, gewijzigd of gearchiveerd kunnen worden. De nieuwe versie van FOCUSPEARL is gekoppeld aan FOCUSSPIN versie 3.3.

1 Introduction

The pesticides used in agriculture are mainly applied to soil-plant systems, e.g. cropped fields. Subsequently, they are subjected to various processes which determine the course of the concentration in the system and the emissions from the soil-plant system to the other environmental compartments. For the evaluation of the risk of leaching to groundwater (as the main source of drinking water) and the exposure of soil organisms to plant protection products pesticide fate models have been developed to support the exposure assessment using the FOCUS scenarios for groundwater (FOCUS, 2000; European Commission, 2014) and the EFSA scenarios for PEC soil (EFSA, 2017).

In the late nineties, the Dutch authorities asked for a model simulating the behaviour of pesticides in soil-plant systems and their emissions from these systems, that could be used as a standard model in pesticide regulation. The new model had to be based on consensus by the most-involved research institutes, i.e. the National Institute for Public Health and the Environment (RIVM, Bilthoven) and Alterra (Wageningen). This new model, i.e. FOCUSPEARL version 1.1.1, was later adopted as one of the models that could be used to evaluate the leaching of plant protection products at the EU level. It consisted of a user-friendly interface, a database containing the data for the FOCUS groundwater scenarios and the SWAP and PEARL model kernels. Since the first release in 2001, updates for FOCUSPEARL have been released, FOCUSPEARL v 2.2.2 in 2003 and FOCUSPEARL v.3.3.3 in 2006. In the subsequent years, the FOCUS groundwater scenarios have been revised and these scenarios have been implemented in FOCUSPEARL v. 4.4.4, which was released in 2011.

During the past years guidance has been developed to assess the exposure of soil organisms (EFSA, 2015, EFSA 2017). The resulting scenarios for the exposure of these organisms, the PEC-Soil scenarios, have been integrated into a new version of FOCUSPEARL, i.e. version 5.5.5. The groundwater scenarios in this version are the same as those in FOCUSPEARL version 4.4.4, except that a few errors have been corrected. These corrections are related to the crop parameterization of onions in the Porto and Thiva scenarios. Further, the irrigation option for permanent crops in the groundwater scenarios has been changed from "Sprinkler_Weekly" to "Surface_Weekly" to bring them in line with the irrigation option for these crops in the soil exposure scenarios.

The current document gives a description of the new version of FOCUSPEARL 5.5.5 and provides guidance to the user how to perform calculations for the assessment of the leaching to groundwater and the exposure of soil organisms. The new version of the FOCUSPEARL database does no longer contain the data on the physico-chemical properties of the compound. Instead, the new FOCUSPEARL version is coupled to SPIN (Substance PlugIN) version 3.3 to enter, edit or archive all substance data needed for a FOCUSPEARL 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 (2020).

The manual consists of three parts. In Chapter 2, the Graphical User Interface is described with reference to the input parameters in the PEARL input file. The Graphical User Interface gives easy access to the most important components of FOCUSPEARL, such as the generation of input files, model execution, output processing and generation of the most important output maps and tables. In Chapter 3 the use of the FOCUS Groundwater scenarios is explained and in Chapter 4 the use of the EFSA soil exposure scenarios. Most users will use only the Wizard functionality to perform assessments of the leaching to groundwater and the exposure of soil organisms.

1.1 Release versions of FOCUSPEARL

The FOCUSPEARL versions can be downloaded from the FOCUS DG SANTE website of the Joint Research Centre in Ispra (Italy) via https://esdac.jrc.ec.europa.eu/projects/pearl. The FOCUS DG SANTE website is the one and only definitive source of the currently approved version of the FOCUS

scenarios and associated models and input files. On the download tab the latest version of the FOCUS PEARL model as well as older versions of the model can be downloaded.

1.2 Compatibility

FOCUSPEARL version 5.5.5 is not compatible with previous versions of FOCUSPEARL, since the substance related data have been taken out from the database and transferred to a separate application SPIN, that has to be used to enter, edit and archive properties of the substances for which the FOCUSPEARL model is to be applied.

To import data on substances as defined in FOCUSPEARL 4.4.4 into the SPIN database version 3.3, a separate application has been developed. This application and a document containing instructions how to use it can be downloaded from the FOCUSPEARL website.

FOCUSPEARL version 5.5.5 has been tested on Windows 7 64 bits and Windows 10 64 bits platforms. The new version supports the use of multiple cores to execute the assessments. Before the start of FOCUSPEARL runs, the interface checks how many cores are available and keeps one available for other processes on the computer. All other cores can be used for the distribution of the PEARL model runs of the assessment.

2 Introduction to the FOCUSPEARL User Interface

This chapter gives an overview of the FOCUSPEARL user interface, which is an integrated environment for data storage and data retrieval, model control and viewing the output data (Figure 2.1). Basically, the user can access the system through the user interface. The user interface is linked with a relational database for easy data access. The user interface generates the input files for the PEARL model and calls the model. Summary outputs are transferred back to the FOCUSPEARL database where they can be accessed. More comprehensive model outputs (particularly time-series) can be viewed with a separate graphical program, XYWIN.
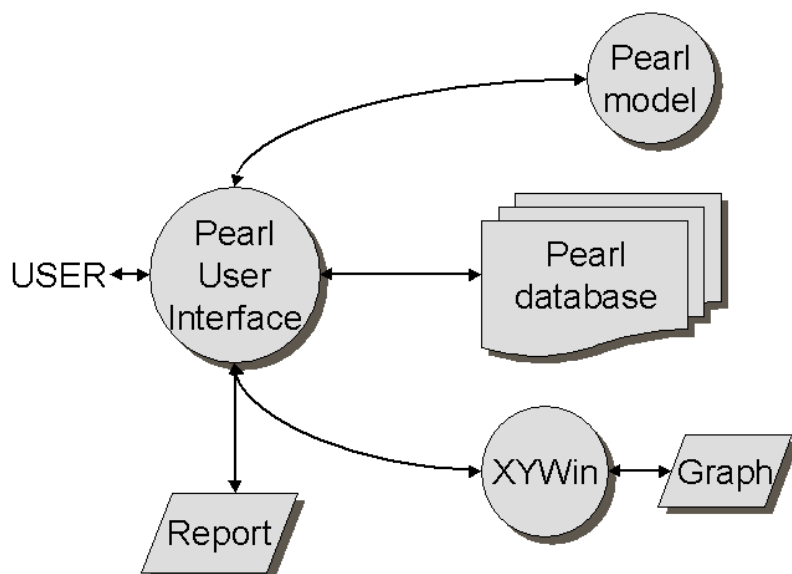
Figure 2.1   *Overview of the FOCUSPEARL modelling system.*

The FOCUSPEARL User Interface makes it easy to:
- organize and edit additional data in the FOCUSPEARL database
- import weather data in the FOCUSPEARL database
- access the scenarios for groundwater and soil organisms
- select one or more model-runs for execution
- perform one or several model runs
- display summary reports containing annual water and mass balance and the target output of the run, either the 80th percentile of the leaching concentration in soil or one of the required concentrations in the soil or in the pore water.
- display model results graphically
- import graphs in Word processor files, using e.g. enhanced Windows metafile format (.emf).

2.1 Overview of the FOCUSPEARL database

As described in Chapter 1, the model will primarily be used in combination with the groundwater or soil exposure scenarios. The groundwater scenarios have been developed for 9 locations and approximately 14 crops per location (FOCUS, 2000; European Commission, 2014). The soil exposure scenarios have been developed for the EU regulatory zones (North, Central and South) for either the total content of the ecotoxicological relevant layer or the pore water concentration in this layer (EFSA, 2017).

The large number of scenarios and model inputs required for one model run leads to a large amount of data. It is clear that organization of all the data is important to i) establish a hierarchy, (ii) minimize data redundancy, and (iii) optimize the data accessibility. An efficient way of handling the data is to use a relational database.

Figure 2.2 shows the hierarchy within the FOCUSPEARL database. The highest level of the database (level 1) is the project level. Here, the user can group several model runs, based on a common criterion (e.g. all model runs for one single field-study or all model runs for one single pesticide). The second level is the model run level. Parameters needed to perform a model run are scenario data, pesticide data, the annual application schedule and the model controls, such as the begin and end time of the simulation. These three major building blocks of a model run are stored at level 3.
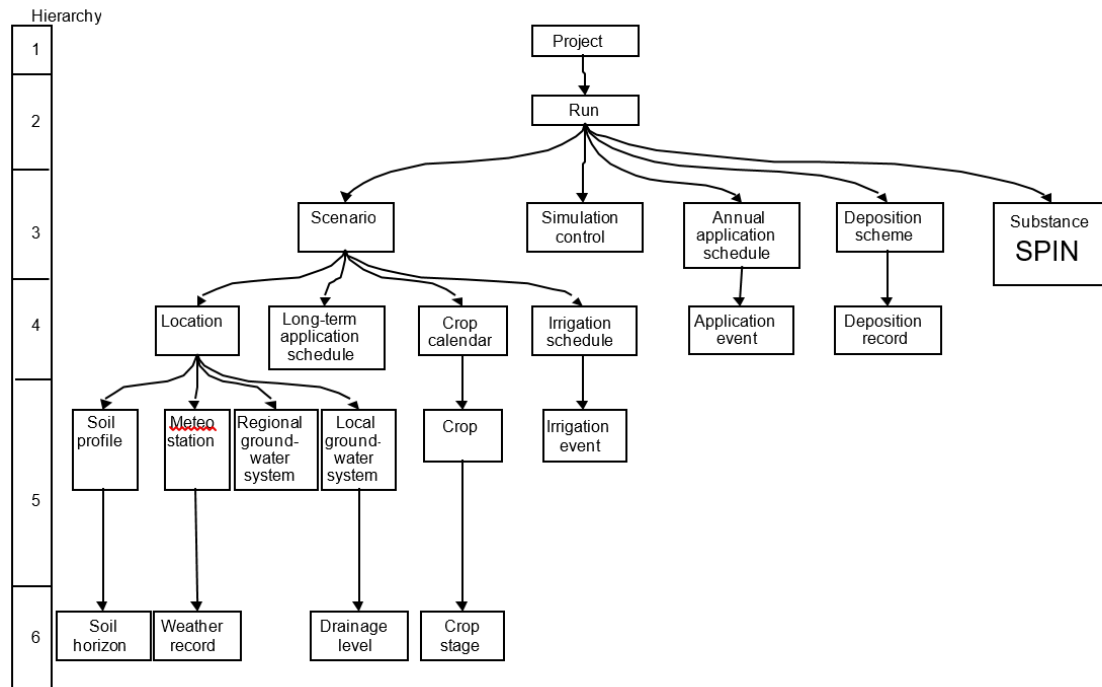
Figure 2.2   *Overview of the FOCUSPEARL database.*

The left hand side of the diagram shows the building blocks of the FOCUS scenarios. These scenarios are a combination of crop, location, the long-term application schedule (i.e. annual, biennial or triennial applications) and agronomic parameters (particularly irrigation data) to be used in the simulation. Parameters referring to a location can be further classified into soil parameters, weather data, parameters describing the regional groundwater system (i.e. the lower boundary of the hydrological model) and parameters describing the local groundwater system (i.e. water flow to ditches and field drains). Note that in the PEARL context, the crop calendar does not relate to a location. Instead, it is one of the building blocks of a scenario, which is at a higher hierarchical level. As shown in the figure, the crop calendar relates to individual crops. The crop calendar may refer to one single crop (monoculture) or several crops. At the lowest hierarchical level are the basic data, relating to a single crop stage, a single soil horizon, etc.

The right hand side of the diagram contains the pesticide data, *not* including application schedules. The pesticide entry is only used to refer to the name of the compound that has been applied (the parent compound), the actual data are entered in the SPIN database. Using SPIN, the compound data are entered into tables containing data on general compounds properties, sorption parameters, diffusion parameters and crop interaction parameters. For a compound with one or more metabolites, the data on the transformation scheme are also entered and stored in SPIN. More details on the use of SPIN are given in the SPIN manual (Van Kraalingen et al., 2020). It should be noted that when

starting SPIN by clicking the Substance button in FOCUSPEARL 5.5.5, only substance data required for runs using FOCUSPEARL need to be entered.

The application schedule and pesticide deposition data are both pesticide and location dependent. This table relates to the table describing the individual application events, which contains information about such parameters as dosage, application mode, application date, etc. As the annual application schedule cannot be directly linked with the pesticide or location tables, they are directly linked with a model run (level 2). The long-term application schedule (i.e. whether a pesticide is applied annually, biennially or triennially) is part of a scenario (FOCUS, 2000; European Commission, 2014).

All other parameters can be accessed through the 'simulation and output control' entries. Here parameters are listed such as start-time of the simulation, minimum time-step, output options, etc.

2.2 Overview of the user interface

After installation of FOCUSPEARL 5.5.5 and the required substance application FOCUSSPIN 3.3, FOCUSPEARL can be started by clicking on the FOCUSPEARL 5.5.5 icon on the desktop or laptop or select the FOCUSPEARL program using the search function for programs or apps. The main screen as presented in Figure 2.3 is shown on the screen.
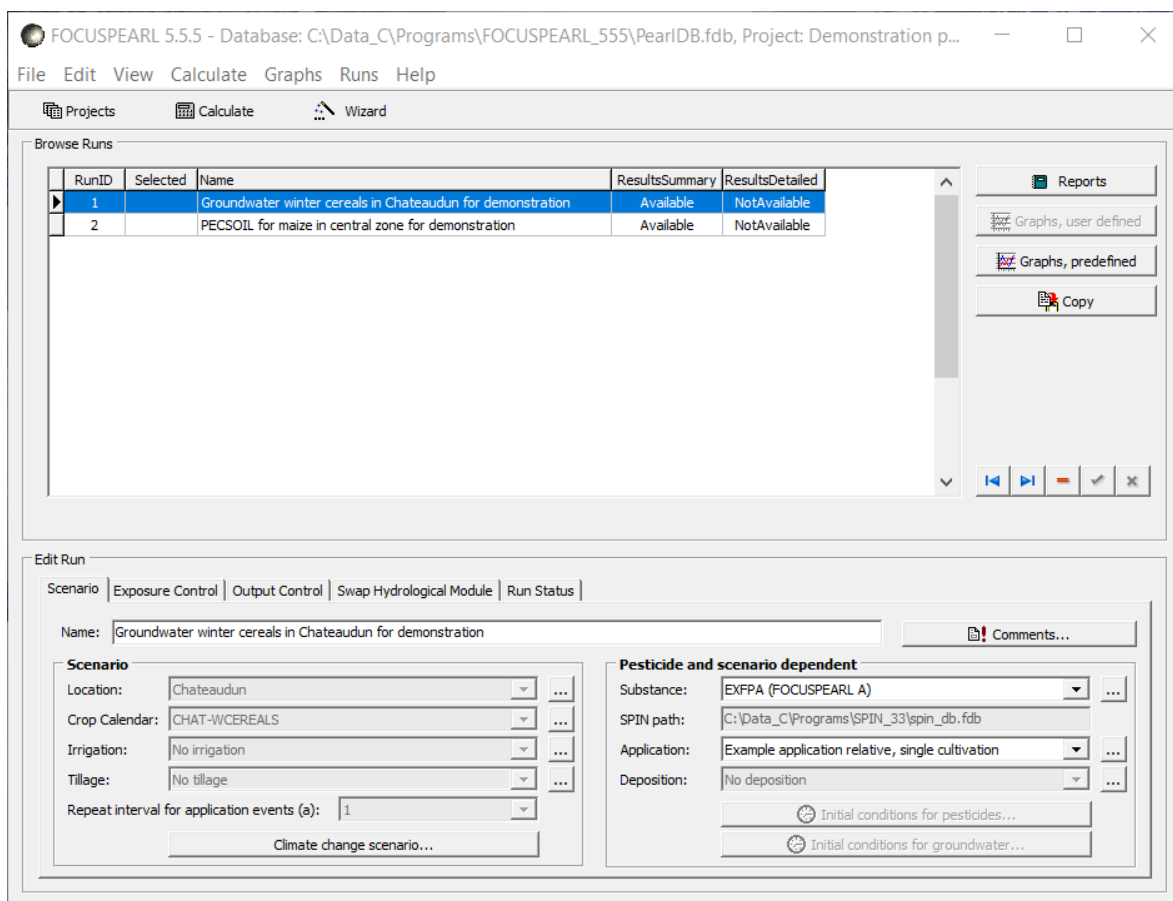
Figure 2.3 *Main screen of FOCUSPEARL 5.5.5.*

On top of the main screen three buttons are shown, the 'Projects', 'Calculate' and 'Wizard' buttons. The 'Projects' button is to allow the user to open the Projects form. On this form the user can add or edit projects. An appropriate description can be added in the 'Description' field of the edit section of the Project form. Additional information can be entered after clicking on the 'Comments' button.

The Calculate button is necessary to start the runs of the project shown that have been selected for execution. The Wizard button has been added to make it easy the user to generate the runs required

using the groundwater or soil exposure scenarios. The use of the Wizard is explained in more detail in Chapter 3 for the Groundwater scenarios and in Chapter 4 for the soil exposure scenarios.

The browse section of the main screen allows the user to scroll through the records of a table (in this case runs). Please note that the information in the edit part changes when scrolling. At the bottom section of the BROWSE part a navigator bar is shown with the following buttons:

⏮	Go to the first record in the table
⏭	Go to the last record in the table
➕	Add a new (empty) record
➖	Delete a record
✔	Confirm changes ('post edit')
✖	Cancel changes

It should be noted that no '+' button is included on the navigator bar to add a run, because the Wizard function has been implemented to add runs.

In the edit section of the main screen the elements describing the run are shown. These are:
- Location
- Crop calendar
- Irrigation
- Tillage
- Substance
- Application
- Deposition

For each of these elements a button ⋯ is shown. After clicking on this button the form is shown for this element. These forms are presented in the next section. The main menu can be used for quick access to various parts of the FOCUSPEARL user interface:
- Use File-Exit (ALT-F-X) to quit the application.
- Use the Edit menu (ALT-E) to directly access a table in the database. As an example, use Edit-Substances or ALT-E-S to jump to the substances form.
- Use the View menu (ALT-V) to view the PEARL input and output files.
- Use the Calculate menu (ALT-C) to execute selected runs.
- Use the Graph menu (ALT-G) to jump to the graphs section.
- Use the Help menu (ALT-H) to access the help file.

The edit section of the main screen consists of five tabs, i.e. the Scenario tab, the Exposure Control tab, The Output Control tab, the Swap Hydrological Module tab, and the Run Status tab. In the next sections, the labels mentioned between brackets refer to the labels as used in the PEARL input file. A detailed description of all input parameters for the PEARL model is presented in Annex 1.

Scenario tab
On this tab, the user has to select the major building blocks of a scenario, i.e. the location, the crop calendar, the irrigation scheme, the (parent) pesticide (substance), the application scheme and the deposition table. The application scheme gives access to tables of application dates. Also the repeat interval of applications (in years) must be specified (DelTimEvt). If set to 2, for example, biennial applications are simulated. If set to NoRepeat, the application table will not be repeated. The initial conditions of pesticide in the equilibrium domain (ConSysEql) and the non-equilibrium domain of the soil system (ConSysNeq) can be specified in the initial conditions form, which is accessible by clicking on the 'initial conditions button'.

It should be noted that only building blocks available in the database can be selected. Therefore, it may be necessary to add new crops, locations, etc to the database before proceeding. This can be done by clicking on the button to the right of the pick lists to go to a lower hierarchical level. It is also

possible to use the <u>E</u>dit menu of the main menu or use key shortcuts (e.g. ALT-E-C to go directly to the crop calendar).

Exposure Control tab
This section contains general options for the simulation run. The time-domain for the simulation is specified in the Start and Stop date fields (TimStart and TimEnd). The date-format specified at page can be used. Please note that the time-domain is fixed if a FOCUS scenario has been selected. According to guidelines of FOCUS (2000) a FOCUS run should start at 1-Jan-1901. The length of the run is set at 26 years in case of annual applications, 46 years in case of biennial applications and 66 years in case of triennial applications.

The Output Control tab
This section contains items that need to be specified in order to obtain the output in the required format. For the format of the time column of the PEARL output file the following options are offered:
- Number of days since the start of the simulation
- Number of days since 1900
- Years

Using the Print method option the available options for the time interval for the output are: Year, Month, Decade, Day, Hour, Other. If 'Other' is selected the user can specify the print interval in days in the box next to the Print Method option.

For the soil exposure scenarios the top and bottom boundary of the soil layer for the ecotoxicological assessment have to be specified. Other output options are 'Detailed output' and 'Output cumulatives'. If the checkbox for detailed output is selected, then output will be written to the .out file using the file format specification selected on this tab. By default the option for 'Output cumulative' is switched on, which means that amounts of the substance transformed, leached, etc. are reported in the .out file as cumulative amounts. If this checkbox has not been selected, then the amounts relate to the print interval. For example, mass or volume fluxes on a daily basis will be written to the .out file if the print method selected is 'Day'.

The Swap Hydrological Module tab
For runs created with the Wizard for the groundwater runs or the soil exposure runs, only one option can be changed: Option Hydrology. The hydrology option (<u>OptHyd</u>) defines how SWAP is run. The following options are available:
- Run SWAP if there is no existing SWAP output. This option saves computation time.
- Creates input for SWAP only.
- Assumes that SWAP has already been run; a bfo file must be provided.
- Runs SWAP and then PEARL. SWAP will always be run.
- Runs SWAP only (output in PEARL format). This option is interesting when testing or calibrating the hydrological model, without (yet) running the pesticide part.

For runs generated by the use of the Wizard button, other items in this section have been greyed out because default values are used for the groundwater and soil exposure scenarios. The minimum and maximum time-steps in the hydrological model swap (DelTimSwaMin and DelTimSwaMax). These variables determine the minimum and maximum time-steps in the swap model. The model will look for the optimal time step between the pre-set limits. Making the time-step too large could lead to instability, while making it too small will increase the computation time substantially. The tolerance of the iteration procedure (ThetaTol) defines the accuracy of the simulations. Choosing a too large value could introduce a numerical water balance error. The initial groundwater level (GrwLevIni) is also specified in this tab, because it is dependent on the start time of the simulation. It should be noted that other input parameters for SWAP are included in several other forms, such as the 'Soil Profiles' form (see Section 2.3.2).

The Run Status tab
On the 'Run Status' tab information is given on the characteristics and the status of the Run. The RunID is listed and what the status of the Summary and Detailed results is: 'Available' or 'NotAvailable'. The creation and modification dates of the run are also presented on this tab.

2.3 Editing locations

After clicking on one of the ⋯ buttons next to the run elements on the 'Scenario' tab in the 'Edit run' section of the main screen, a form with detailed data on the specifications for this element is shown.
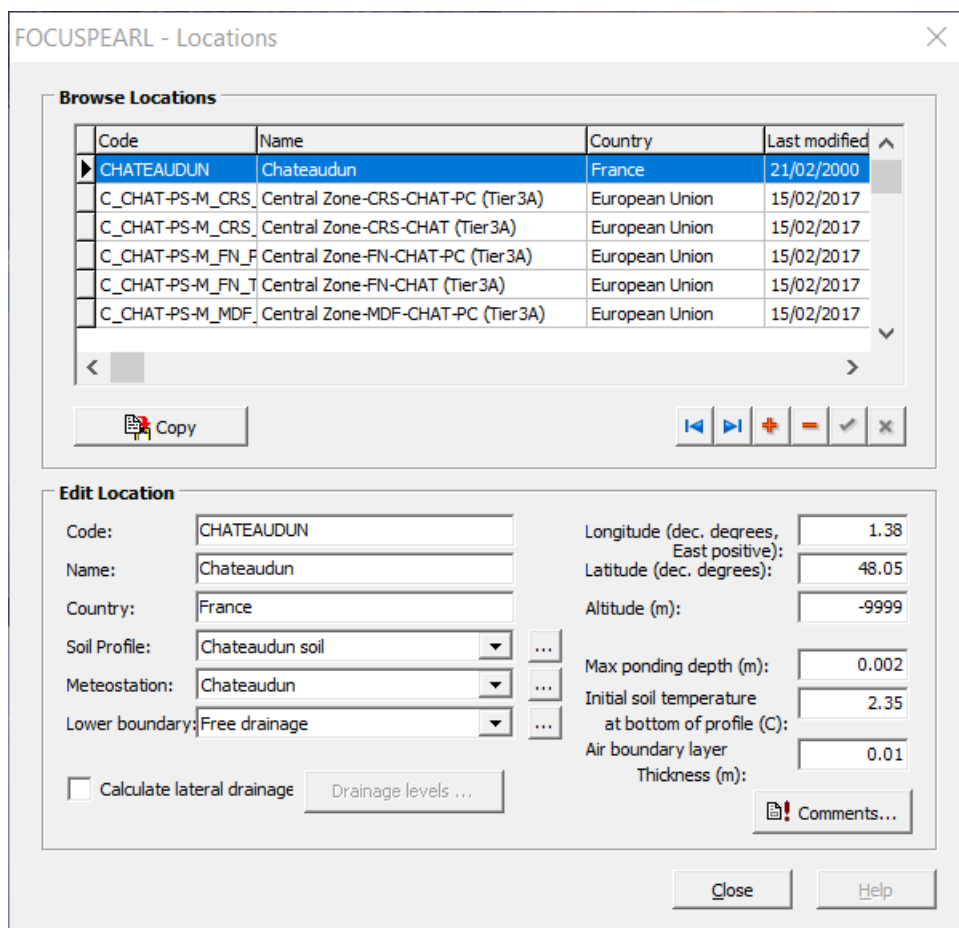
In the edit section of the form there are three categories of data fields:
- ordinary data fields, where a text string, a date string or numerical data can be entered. The PEARL user interface will perform range checking after the data have been entered.
- option fields or pick lists, where a choice can be made between a number of options. The button to the right of a pick list allows to edit the underlying tables (i.e. go to a lower hierarchical level).
- check boxes, where variables can be switched on or off.

Most forms are complemented with a comments button, which allows to add additional information or meta-data if needed.

2.3.1 The Locations form

After clicking on the ⋯ button on the right-hand side of the Location box on the main screen, the form presented in Figure 2.4 is shown. In the upper section of this form all the available locations in the FOCUSPEARL 5.5.5 database are listed. Upon selection of one of these locations, the data on this location are shown in the 'Edit Location' section of this form.

Figure 2.4   *The Locations form.*

In the 'Edit Location' section of this form general information on the site is given, such as the name and the altitude. The locations form can be accessed from the scenario tab of the main form, but the user can also use the edit menu of the main form. In the 'Edit Location' part a soil type and a weather station have to be selected. Please note that only one of the available soil types or weather station can

be selected. To select a new soil type or weather station, a new soil type or weather station need to be created first on the 'Soil Profiles' form or the 'Meteo Stations' form, respectively.

From the Locations form the user has access to data that are usually spatially distributed, such as soil data, weather data and information about the local and regional groundwater system. Exceptions are the crop calendar and the irrigation schedules, which are at higher hierarchical levels according to definitions by the FOCUS (2000).

An option for the lower boundary condition of the hydrological model must be selected in the Lower Boundary Condition pick list (OptLbo). SWAP offers eight options for the lower boundary condition. For several of these conditions parameter values must be introduced in the lower boundary conditions form, which can be opened by clicking on the ⋯ button. On this form the option is given to include drainage by selecting the 'Calculate Lateral Drainage' checkbox (OptDra). Then the 'Drainage Levels' button can be used to get access to the form with the data needed for different drainage levels. For FOCUS groundwater and EFSA PEC Soil runs no drainage is considered. Therefore, the 'Calculate Lateral Drainage' checkbox is not selected and it cannot be changed by the user.

On the Locations form itself, the user must specify a unique code for the location, the location name and the country name. The altitude (Alt), longitude and latitude (Lat) are also required. Positive numbers refer to locations in the Eastern and Northern Hemispheres, respectively. The initial soil temperature (°C), which is used to initialize the soil heat flux submodel must also be specified here. Further, the maximum ponding layer depth (ZPndMax) must be specified, which determines the maximum thickness of the water layer that can be present on the soil profile before surface runoff starts. The thickness of the air boundary layer must be specified in the ThiAirBouLay record. This parameter is relevant for the calculation of surface volatilization of pesticides.

2.3.2 The Soil Profiles form

The Soil Profiles form consists of two parts as is shown in Figure 2.5. The 'Edit Soil profile' section of this form contains parameters that apply to the soil as a whole, whereas in the 'Edit Horizon in Soil' section the user can introduce properties of individual soil horizons.

Figure 2.5 *The Soil Profiles form.*

In the 'Edit soil profile' section of the soil profiles form, the user must specify parameters that apply to the soil profile as a whole. First, specify a unique code and a name for the soil profile.

In the relative diffusion pick list, one of the functions for the calculation of the relative diffusion coefficient (OptCofDifRel) must be chosen. Three options are offered, i.e. the functions published by Millington and Quirk (1960), Currie (1960) and Troeh *et al* (1982)*.* The actual parameters of these functions must be introduced in the 'relative diffusion function', which is accessible with the button to the right of the relative diffusion pick list. More information on the parameterization of the relative diffusion function is presented in Van den Berg et al. (2016).

The actual soil evaporation rate is calculated using hydraulic properties and an empirical reduction function. Parameter β of the Boesten relationship must be provided in the CofRedEvp field The potential evaporation calculated corrected by a factor FacEvpSol, see Boesten and Stroosnijder (1986) for more details. This is particularly important in the case of a small soil cover fraction, because this equation has been derived for situations where the canopy shades the ground. FacEvpSol can be given a value between 0.5 and 1.5.

If the bulk density is unknown, it can be calculated by the model. In this case, the bulk density option (OptRho) should be set to calculate. See Bollen et al. (1995) for details on the pedotransfer function used. If observed values on the bulk density are available, then these values can be introduced.

In Edit Horizon in Soil part the user has to specify the vertical discretization of the soil profile (i.e. the SoilProfile table). Soil horizons can be added by using the '+' button of the navigator.

The user must specify the thickness of each soil horizon and the number of compartments used in the finite-difference scheme. For each horizon, the user must also specify a soil building block, which contains information on basic soil properties and hydraulic properties. If the appropriate soil building block is not yet available, then this soil building blocks form has to be entered before editing the soil profile. The number of soil compartments is a compromise between accuracy and computation time. Computation time increases approximately with the square of the number of soil layers. On the other hand, predictions may become inaccurate if the layer thickness is taken too large. This is particularly true if the expected concentration in the groundwater is lower than 0.001 µg L^{-1} (Van den Berg et al., 2016). A layer thickness ranging from 1.0 cm in the top 30 cm up to 10 cm in the layer below 1 m may be a fair compromise.

The dispersion length, Ldis (LenDisLiq) is entered directly in the soils screen (and not in the soil horizon screen), because it is considered a soil property that is not coupled to generic soil horizons. Please note that the distance between the nodal points, Δz, should be small enough (see Van den Berg et al. 2016, Chapter 11).

Factors for the effect of depth on transformation (FacZTra) and sorption (FacZSor) are also specified in the soil screen. The factor for the effect of depth on sorption is only relevant if the option for the calculation of Freundlich equilibrium sorption in the substance screen is set to CofFre. This factor must be 1.0 for the top-soil.

2.3.3 The Soil Building Blocks form

For each soil building block, the basic soil properties (SoilProperties) and soil physical parameters have to be specified.

In the upper section of the form as shown in Figure 2.6, the textural distribution (FraSand, FraSilt and FraClay), the mass content of organic matter (CntOm), the pH and the bulk-density (Rho) have to be specified. Note that the textural distribution refers to the mineral part of the soil only, so the sum of the sand, silt and clay fractions should be equal to 1.0. The mass content of organic matter refers to dry soil. The *p*H is used for the sorption model of weak acids. As most sorption experiments are being carried out in 0.01 *M* CaCl$_2$, the *p*H-CaCl$_2$ is preferred. If the *p*H-CaCl$_2$ is not available, the pHCorrection variable in the substance screen should no be equal to zero. On the form itself 'pH-H$_2$O' is listed, but there is no requirement that only pH-H$_2$O values can be entered. The bulk density is only required if the option for the calculation of the bulk density in the soils screen has been set to 'Input'.

Figure 2.6   *The Soil Building Blocks form.*

In the lower half of the form, the user has to introduce the parameters of the Mualem-Van Genuchten functions. Values on θ_s (ThetaSat, θ_r (ThetaRes), α (AlphaDry and AlphaWet), n (n), K_s (KSat) and λ (l) need to be introduced. The parameter AlphaWet is only relevant if the option to take hysteresis into account has been selected.

2.3.4   The Meteo Stations form

The Meteo Stations form is shown in Figure 2.7. The user has to specify information about the weather station. First, the user must specify a unique code for the weather station (MeteoStation). Please note that this code may not exceed eight characters. The altitude (Alt), longitude and latitude (Lat) are also required.

The potential evapotranspiration can be obtained in different ways. The user must specify one of the available methods in the evaporation options field (OptEvp). Three options are available: (i) the potential evapotranspiration is input by the model, (ii) the Penman-Monteith equation is used, and (iii) the Makkink equation is used. If Penman-Monteith is selected, solar radiation, minimum and maximum air temperature, air humidity, wind speed and precipitation are required. If Makkink is selected, only minimum and maximum air temperature, solar radiation and precipitation are necessary.

Weather data from other weather stations can be imported into the FOCUSPEARL database. Before starting the import of the weather data, the meteo station code as specified in this file should already be available in the list of Meteo stations. The format of the file with weather data is described in Annex 2.

Figure 2.7 *The Meteo Stations form.*

2.3.5 Boundary conditions of the hydrological model

SWAP makes a distinction between the seepage flux due to regional groundwater flow and the local drainage flux to ditches and field drains. The seepage flux due to regional groundwater flow is the lower boundary condition of the model, and must be defined in the lower boundary conditions form, the local drainage flux is considered a sink term and must be defined in the drainage levels form.

The SWAP model offers eight options for the lower boundary condition, which must be specified in the locations form. Most options require additional input, which must be specified in the lower boundary conditions form. Depending on the option chosen, only the relevant tab is shown. Data fields on other tabs may be edited, but only the data on the option selected are used in the simulation.

If the lower boundary condition is set to 'time dependent groundwater level', the groundwater level must be specified as a function of time (table GrwLev). Normal data-format can be used.

If the lower boundary condition is set to 'flux boundary condition', a sine function is applied to generate the daily regional bottom flux. The user should specify the mean (FlvLiqLboAvg) and amplitude (FlvLiqLboAmp) of the annual bottom flux. Also the date at which the maximum of the sine wave occurs should be given (DayFlvLiqLboMax). Note that negative values denote downward fluxes and positive fluxes denote upward values.

If the lower boundary condition is set to 'flux from deep aquifer', the regional bottom flux is calculated using the head difference between the phreatic groundwater and the groundwater in the semi-confining aquifer. The average groundwater level in the field, Φ_{avg}, is affected by the drainage base (HeaDraBase) and by the shape of the groundwater table (OptShapeGrwLev), which can be Elliptic, Parabolic, Sinusoidal or NoDrains. The daily value of the hydraulic head in the semi-confining aquifer, Φ_{aqf} is described by a sine-wave. Then its annual average value (HeaAqfAvg, the amplitude (HeaAqfAmp) and the date at which the maximum hydraulic head occurs (TimHeaAqfMax) must be specified. The bottom flux eqn. is also affected by the vertical resistance of the aquitard (RstAqt, γ_{aqt}). See Kroes et al. (2008) for more details.

If the lower boundary condition is set to 'groundwater-level-drainage relationship', the bottom flux is calculated as a function of the groundwater level. If this option is chosen, the model needs the coefficient (CofFncGrwLev) and the exponent (ExpFncGrwLev). Please realize that this option is only valid for deep, sandy areas. The calculated bottom flux includes local drainage to surface waters and drains, so local drainage should be set to zero if this option is used.

If the lower boundary condition is set to pressure head boundary condition, the pressure head at the lower boundary should be specified in cm as a function of time (table h). Normal date format can be used (dd/mm/yyyy).

The FreeDrain, Lysimeter and ZeroFlux options do not require additional input.

If the lower boundary condition of the hydrological model is set to 'groundwater level as a function of time', 'flux boundary condition', 'flux from deep aquifer', 'pressure head boundary condition', or 'zero flux', a local drainage flux can be defined in addition to the regional seepage flux. First check the 'calculate local drainage' box, then enter the 'drainage levels screen'. Use the '+' sign of the navigator to add drainage levels. Up to five local drainage level systems can be specified.

For each local drainage system, a drainage flux is calculated. The model needs information about the bottom of the drainage system (ZDra) and the drainage resistance (RstDra). The procedure that distributes the drainage flux over the individual soil layers additionally requires information about the drainage type (DraTyp) and the distance between the drainage systems (DistDra). The user should also specify whether the local drainage system is a field-drain or an open channel.

2.4 Editing crop calendars

From the crop calendar form the user can access the data on the crop rotation, parameter values for individual crops and crop stages. The crop calendar is accessed directly from the scenario screen, because it is one of the main building blocks of a FOCUS scenario (FOCUS, 2000). PEARL uses a simple crop growth model, i.e. relevant crop parameters such as the Leaf Area Index and rooting depth have to be provided as a function of development stage (see below).

2.4.1 The Crop Calendar form

The definition of the crop calendar (table Crops) starts in the Crop Calendar form, which is accessible from the scenario tab of the main form. This form is presented in Figure 2.8. The crop calendar should be given a unique code and a name. It is very important to specify whether the same crop calendar must apply to all years (option RepeatCrops) or whether separate crop calendars are used for individual years.

The course of development stage with time can be defined by selecting 'Fixed' for the option OptLenCrp or it can be controlled by the temperature sum by setting the option OptLenCrp to 'Variable'. The advantage of defining the crop development stage dependent on the temperature sum is that regional differentiation of crop growth can be made on the basis of air temperature.

Crops can be added to the crop calendar in the browse crops section by clicking on the '+' button of the navigator. It may be necessary to add a new crop before proceeding. In this case, first go to the crops screen (see below). The emergence date (this is later than the date of seeding) and the harvest date are defined directly in the crop calendar page, all other crop parameters are entered on the 'Crops' form. Please note that a single crop can occur several times in the crop calendar, but a single crop is linked to one crop development stage table (see below). If the crop has different development stages over the years, a unique crop name must be specified for each year, e.g. Maize01, Maize02, etc. During periods that no crop is present, the model will use parameter values for bare soil.

Figure 2.8   *The Crop Calendar form.*

2.4.2   The crops and crop stage form

The Crops form can be accessed using the [...] button next to the crop pick list, in the Crop calendar form (see above). In the Crops form, all time-independent crop properties are input, as shown in Figure 2.9. Dynamic crop properties are input in the crop stages form.
The user must enter the pressure heads defining the root water extraction function: HLim1 is the anaerobiosis point, HLim2 is the reduction point at near-saturation, HLim3U is the reduction point at dry conditions and at low evaporative demand, HLim3L is the reduction point at dry conditions and at high evaporative demand, and HLim4 is the wilting point (see Feddes et al. 1978). If these values are available for pF values instead of pressure heads, they should be converted according to the $h = -10^{pF}$.

If the Penman-Monteith equation is used for the calculation of potential evapotranspiration, SWAP additionally requires the minimum canopy resistance. The minimum canopy resistance ranges from 30 s m^{-1} for arable crops to 150 s m^{-1} for trees in forests. See Allen *et al.* (1989) for parameter values.

PEARL needs the extinction coefficient of global solar radiation, κ, (see Kroes et al., section 3.4.1). Parameter values for some common crops can be found in section The interception coefficient CofIntCrp controls the amount of interception of water by the crop canopy. In case of ordinary agricultural crops, this interception coefficient may be set to 0.025, see section 3.2.1 in Kroes et al. (2008). If set to zero, no interception will be calculated (in fact PEARL will write a very small value to the SWAP input file for the crop to prevent division by zero). Please note that at high precipitation rates, the interception rate asymptotically reaches a value of a·LAI (Eqn 2.52 in Kroes et al., 2008).
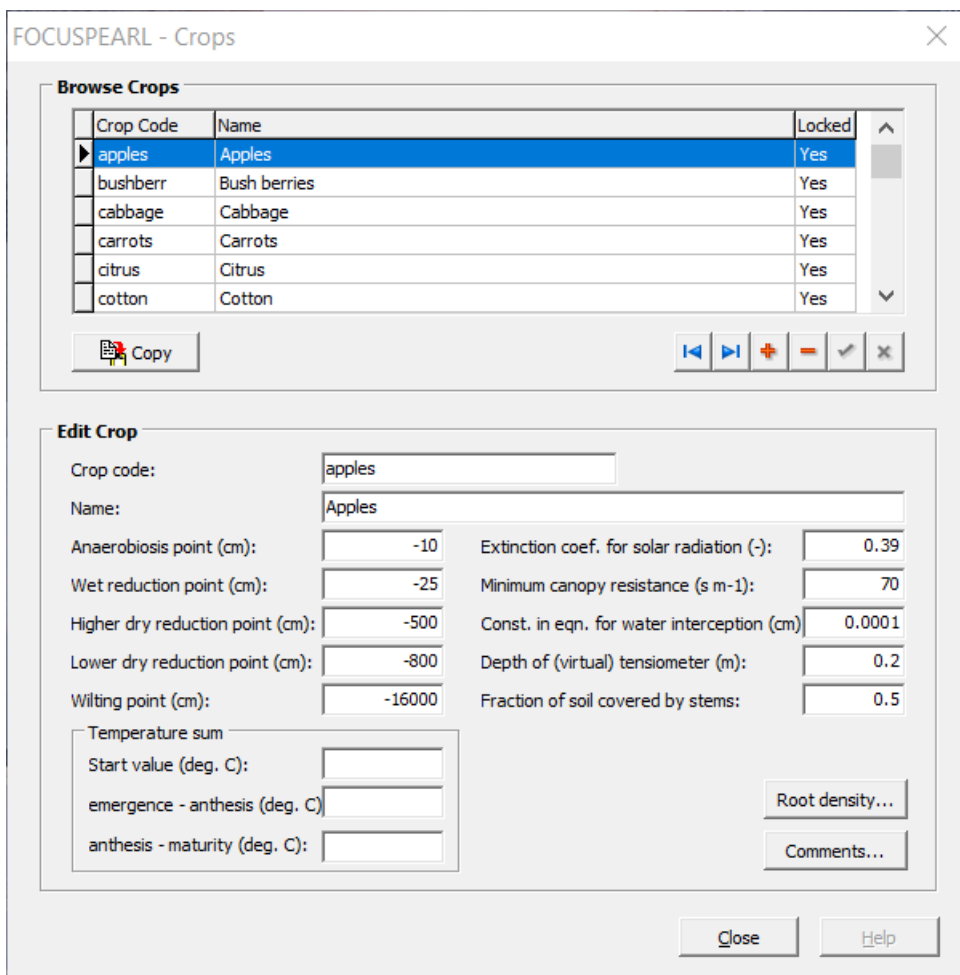
Figure 2.9   *The Crops form.*

The root density is specified in the relative root density form (press the relative root density button). The user may enter up to 11 data pairs to define the relative root density distribution as a function of the relative rooting depth (table RootDensity). Any unit can be used, the model will normalize the root density distribution in such a way that the integral of root density times depth over the root zone equals one.

If the course of development stage was set to 'Variable', the user must specify the temperature sum at emergence (TemSumSta) the temperature sum from emergence to anthesis (TemSumEmgAnt), and the temperature sum from anthesis to maturity (TemSumAntMat).

Dynamic crop properties are input in the 'Crop stages' form (See Figure 2.8), which is accessible through the stages button. These properties are input as a function of the development stage. The development stage is 0 at emergence, 0.5 at flowering (anthesis) and 1 at maturity (note that in the original publication by Van Heemst (1986), the development stage is between 0 and 2). Use the '+' button of the navigator to add development stages. A maximum number of 36 development stages is allowed for each crop.

For each development stage, the Leaf Area Index (LAI) and the rooting depth (ZRoot) have to be specified. If the potential evapotranspiration is calculated according to the Makkink equation, an empirical crop factors must be introduced (FacCrp). If the potential evapotranspiration is calculated according to Penman-Monteith, the crop height must be specified (HeightCrp).

2.5 Editing substances

PEARL 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. Substances can be added by clicking on the ⋯ button next to the 'Substance' field on the scenario tab of the main form. Then a separate application is started called SPIN (Substance Plug IN) and a form is opened which allows to create a new substance or edit a substance that already exist in the SPIN database. Detailed information and instructions how to use SPIN can be found in the user manual for SPIN version 3.3 (Van Kraalingen et al., 2020).

The definition of the transformation scheme, if relevant, can be defined in SPIN too. Further information on how to introduce a transformation scheme is presented in the SPIN manual (Van Kraalingen et al., 2020).

2.6 Editing application schemes

2.6.1 Application schemes

The 'Application scheme' form is accessible from the scenario tab of the main form, because it is considered a major building block of a FOCUS scenario (Applications table). The entire application scheme can be repeated annually, biennially or triennially using the 'repeat interval for applications' option.

Application schemes can be added with the '+' button of the navigator. The user can also copy an existing application scheme. Application schemes should be given a unique code for reference and a description. Use the 'Applications' button to define the individual applications.

2.6.2 Applications

The application form is shown in Figure 2.10. A new application scheme can be added by clicking on the '+' button of the navigator on the left-hand side or copy an existing application scheme using the 'Copy' button. After clicking on the '√' (post edit) button, the data on the applications can be entered in the lower half of the right-hand pane. The date of application can be an absolute date or a relative date, i.e. relative to 'emergence' or 'harvest' of the crop. Next the data for each application can be specified. First define the application type: 'application to the soil surface' (AppSolSur), 'injection' (AppSolInj), 'incorporation' (AppSolTil), 'application to the crop canopy, interception fraction calculated by the model' (AppCrpLAI) or 'application to the crop canopy, interception fraction supplied by the user' (AppCrpUsr). Then enter the date (relative or absolute) and the dosage. For absolute dates the normal date format can be used, i.e. mm/dd/yyyy. A year number has to be entered, but the year will not be used if the repeat interval of applications is set to 1, 2 or 3 (see section 2.2). In the case of injection or incorporation, the incorporation or injection depth must be supplied additionally. Note that an application scheme may contain a combination of applications with relative and absolute application dates.
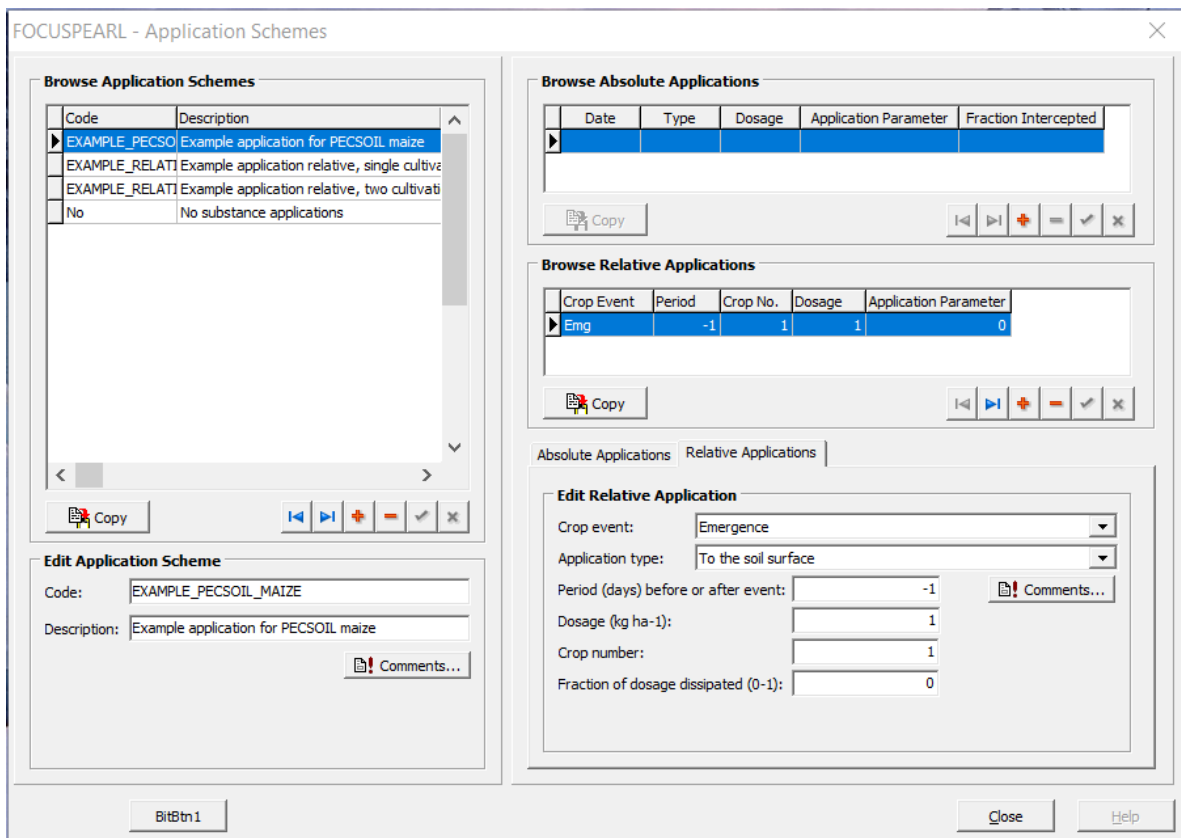
Figure 2.10 *The applications form.*

2.7 Editing irrigation schemes

The irrigation scheme form is accessible from the scenario tab of the main form, because it is considered a major building block of a FOCUS scenario. The irrigation method (OptIrr) can be set using the 'type' pick list of the 'Irrigation Schemes' form.

A new irrigation scheme can be added by clicking on the '+' button of the navigator or copy an existing scheme. The irrigation scheme must then be given a unique code and a description. Two types of irrigation can be specified in PEARL, i.e. sprinkler irrigation and surface irrigation. For each of these two types, irrigation amounts can be predefined by the user or the amounts can be calculated by the model. For the latter case, the option to be selected is either 'Sprinkler irrigation, irrigation depth calculated by the model' or 'Surface irrigation, irrigation depth calculated by the model'. Two options for the calculation method are available. The first option calculates the amount to be irrigated for any day on which the irrigation criteria is met, which is based on the moisture condition in the top soil. For the FOCUS scenarios with irrigation, an alternative option is available. During the growing season the moisture condition is checked once a week. If the amount of water required to bring back the moisture content in the top soil back to field capacity exceeds 15 mm, then irrigation starts. If this amount is less than 15 mm, then no irrigation takes place. However this parameter can be modified when running PEARL in batch mode.

After selecting the option to use predefined irrigation data, the actual irrigation data (IrrTab) must be specified in the irrigations part on the right-hand side of the form. Use the navigator to add a new irrigation event. Both the date (column 1) and the irrigation depth (column 2) should be given. The user can import irrigation schemes from an ASCII file using the 'Import Datafile...' button.

2.8 Defining the output of the model

Before running the model, the user has to define the output that has to be created with PEARL. A default selection of output variables settings has been made and usually this selection will be enough for most purposes. Output is controlled in the output tab of the main form. This tab contains three fields that affect all variables in the output file.

2.8.1 The Output Control tab of the main form

The Output Control tab is shown in Figure 2.11. On this form the user can set the print interval DelTimPrn. The default value for the print interval is 'Month'. The size of the output file can be reduced by setting the print interval to higher values. It should be noted that the output of PEARL is averaged over the print interval and that the time written to the .out file is in the middle of the print interval.

The user can set the depth of the leaching target layer (Ztgt). The user can further set the following switches:
- specification whether the user want to include the detailed output file or not
- specification whether fluxes must be printed cumulative or not.

If 'Detailed output' is selected, specific output variables can be selected on the 'Detailed Output Options' form (see below). This form is opened after clicking on the button 'Detailed output options …'
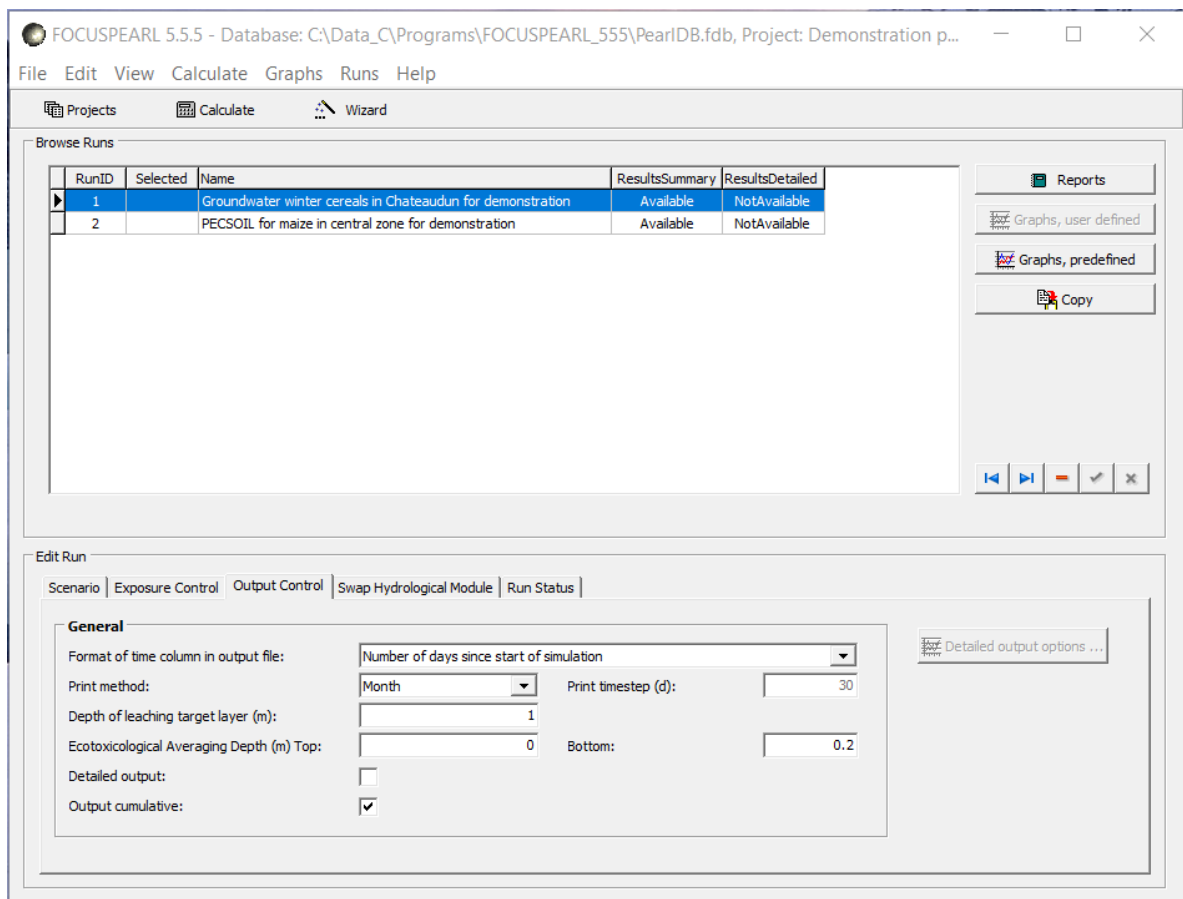
Figure 2.11 *The Output Control tab.*

2.8.2 The Detailed Output Options form

The detailed output options form is accessible from the output control tab of the main form. This form consists of three parts (see Figure 2.12):

- In the upper part the user can browse the categories of available variables.
- In the lower-left section of the form the user can browse the individual variables within a category
- In the lower-right section of the form the intended output depths can be selected.

Figure 2.12   *The Detailed Output Options form.*

PEARL has the following categories of output variables available:
- Pearl balance: Mass balance of the soil system, which includes variables such as the areic mass of transformation and the areic mass of pesticide in the soil system.
- Pearl contents: Concentration of pesticide in the various phases of the soil system, such as the total mass content and the concentration in the liquid phase.
- Pearl crops: Mass balance of pesticide at the crop canopy.
- Pearl fluxes: Mass fluxes of pesticides, such as the total mass flux of pesticide.
- Pearl general: Miscellaneous variables, such as the time-step.
- Swap fluxes: Volume fluxes of water, such as the soil water flux.
- Swap states: State variables of the hydrological model, such as the soil water content.
- Swap general: Miscellaneous variables, such as the groundwater level.

In the lower section of the form, the user can select variables for output. Variables can be switched on and off by double-clicking. It is also possible to use the buttons at the bottom of the form:
- Clicking on the 'TOXSWA Variables' button selects all variables wanted by the TOXSWA model (Horst *et al.*, 2016).
- Clicking on the 'Clear All Variables' button disables all variables.
- Clicking on the 'Set All Variables' enables all variables.
- Clicking on 'Set Defaults' enables the most important model outputs.

Use the '+' button of the navigator key to add additional output depths, use the – key to delete depths. By default, the model will produce output at 5, 10, 20, 30, 40, 50, 75, 100 and 200 cm. Notce that the output depths form applies to all selected variables. Be critical in selecting output depths: more output depths will result in larger output files.

2.9 Running the model

When ready with editing the model input and defining the output variables for the runs in the project, the runs can be selected or deselected for execution. In the column 'Selected' the selection status is shown. After a double click on the box for a run in the 'Selected' column, the selection status can be changed. If not selected then a double click changes the status into 'Yes'. When all runs to be executed have been selected, click on the 'Calculate' button to actually start the model for these runs. If all the runs in the project need to be executed then it is easier to select 'Runs' on the menu bar and select 'Select All runs for execution'. In the Runs menu the user can also deselect all runs for execution.

The first time a run is selected for execution, the PEARL user interface will generate the weather and irrigation data files. This can take some take. PEARL input files will always be generated after clicking on the 'Calculate' button. Next a console window with the logo of the PEARL simulation kernel appears on the screen which shows the progress of the run. The run can be interrupted by entering CTRL-C. The actual computation time depends upon the number of numerical compartments in the soil profile (Van den Berg et al., 2016). Computation time can be reduced by reducing the number of output variables selected for output or reducing the number of output depths (section 2.8.1).

The FOCUSPEARL user interface allows the execution of multiple runs, so there is no need to wait with starting the second run until the first is ready. Furthermore, FOCUSPEARL 5.5.5 supports the use of multiple cores to execute the runs in the project. Before starting the execution, the interface checks how many cores are available on the system and keeps one core available for other processes. All other cores are used for the distribution of the PEARL model runs to be executed. More information on this functionality is given in section 3.2.

When a model run is completed, the user will see the ResultsDetailed, ResultsSummary and Modified columns changing. Possible values for the Results columns are:
- NotAvailable: the model has not (yet) been run or the user has removed the output files
- Error: an error has occurred. Details can be seen in run status tab of the main form.
- Available: the model has successfully been run, and the model output is available for further processing (e.g. the creation of graphs).

2.10 Creating graphs

After a model run has been completed, the output can be analysed via the graphical function of the PEARL model interface. Using FOCUSPEARL a number of predefined graphs can be prepared, but user-defined graphs can also be created. The predefined graphs provide easy access to the most commonly used model outputs, such as the target concentration of pesticide in the groundwater, the areic mass balance of pesticide, etc. With user-defined graphs, the user can view the data in several different ways, which is an useful feature for those users who want to analyse several aspects of the leaching study.

2.10.1 Working with predefined graphs

Predefined graphs can be accessed with the 'predefined graph' button in the main form. The following graphs are available:
- Annual mass balance of the compound in the soil system and the FOCUS target layer, which shows the annual mass balance terms (i.e. annual application, transformation, lateral drainage, leaching, uptake and volatilization).
- Annual water balance of the soil profile and the FOCUS target layer (i.e. annual precipitation, irrigation, seepage, soil evaporation, transpiration and evaporation of intercepted water).
- FOCUS summary graph. The FOCUS summary graphs shows the frequency distribution of the leaching concentration, the 80th percentile of the leaching concentration, etc.

2.10.2 Working with user-defined graphs

PEARL can create graphs of all selected model outputs (see section 2.8.2). The custom graphs form is accessed from the main form. To create a graph perform the following actions:
- Select one of the categories in the upper box.
- Select one or more variables by double-clicking on the variable name in the lower box.
- If the selected variables are depth dependent, one or more depths can be selected by clicking in the output depths box (refer to the HasDepth column).
- If the selected variables are substance properties, one or more substances can be selected in the substances box (refer to the IsCompound column).

The user can plot multiple variables in one graph, but a variable that is depth dependent cannot be mixed with another variable that is depth independent. Click on 'Graph' when ready.

2.10.3 The XYWIN program

FOCUSPEARL uses the graphical program XYWIN. After clicking on the 'graph' button, a message box appears showing the number of selected data-pairs. After a while, the selected graph will be displayed. The user can zoom in with the left mouse button and zoom out to the original size (Edit menu or press F8). This function is not available in predefined graphs.

Graphs can be printed from the XYWIN menu (select Print from the File menu or press Ctrl+P). XYWIN can create output in different formats, such as emf, png, jpg or tiff.

3 Using FOCUSPEARL for the FOCUS groundwater scenarios

FOCUSPEARL supports the application of the FOCUS Groundwater scenarios to assess the leaching of plant protection products to groundwater (FOCUS, 2000; European Commission, 2014). Runs using these scenarios can be prepared with the FOCUS wizard. The FOCUS wizard guides the user through the following steps:

1. Selection of one or more FOCUS crop(s)
2. Selection of one or more FOCUS location(s)
3. Selection of the substance (only parent substances can be selected), the application scheme and the repeat interval for the application scheme (annual, biennial or triennial).

Note that in the FOCUS wizard, the user can only select application schemes or substances that are available in the FOCUSPEARL and SPIN databases, respectively. A new application scheme has to be added to the FOCUSPEARL database first before it can be selected to create runs with the Wizard. A new substance has to be added to the SPIN database first. The FOCUS crops and FOCUS locations have been defined by the FOCUS Groundwater Workgroup and they cannot be edited. Also, the time-domain for the simulations is fixed, depending on the repeat interval of the application scheme.

After running the FOCUS wizard, the user interface has created a new project. Note that a number of combinations are not valid (e.g. vines in Jokioinen), so these will not appear in the project created. The newly created project is a so-called 'fixed substance project', which implies that all runs refer to the same substance. Editing this substance affects all selected runs. As it may be desirable to run the model with different application schemes, each run has got its own application scheme. A plant protection product may be applied in Thiva (Greece) at dates different from those in Hamburg (Germany). The application schemes of the individual runs are copies of the application scheme that has been selected in the wizard procedure.

All runs in the newly created project have already been selected for execution – they can be executed by clicking on the Calculate button. When done, graphs and summary reports can be created.

3.1 The Wizard for the creation of groundwater assessments

After starting FOCUSPEARL, the main screen of the interface is shown. Just below the menu bar three buttons are shown, the 'Projects', 'Calculate' and 'Wizard' buttons. To generate groundwater exposure runs, the following procedure has to be followed:

Step 1: Start the FOCUSPEARL wizard by clicking on the 'Wizard' button. A window appears which gives two options for the wizard, which is shown in Figure 3.1.
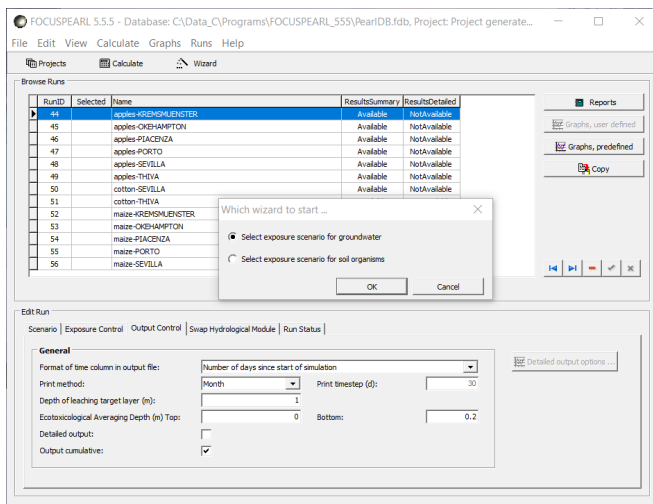
Figure 3.1 *The form to specify the type of Wizard: groundwater or soil exposure.*

Step 2: Select exposure scenario for groundwater and click on the OK button.

Step 3: Select the crop by a double click on 'Apples', 'Cotton', 'Oil seed rape (winter)', 'Maize' and 'Soybean' in the left column or click on the crop name and then click on the '>' button. The result is shown in Figure 3.2. Then click on the 'Next' button.
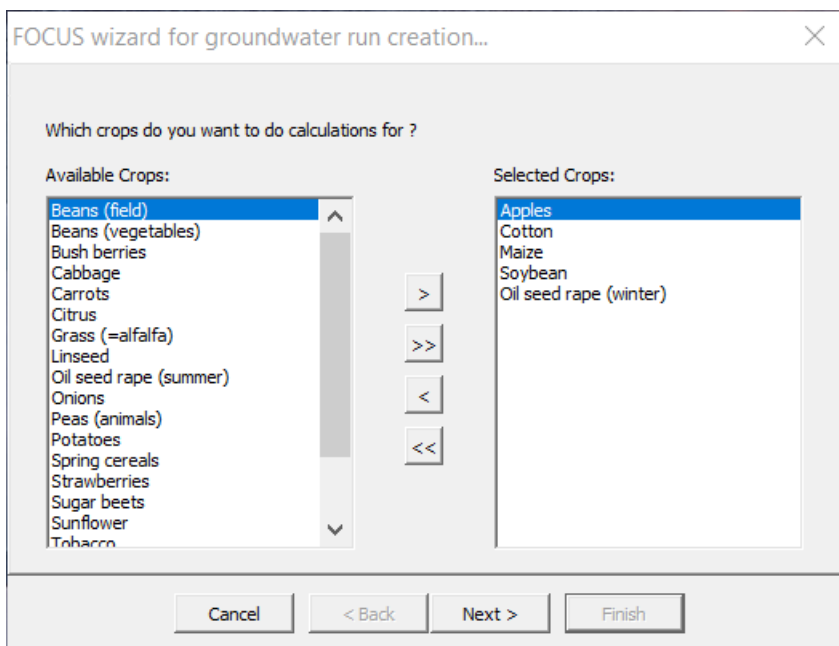
Figure 3.2 *The Groundwater wizard; the selection of crops.*

Step 4: Select the locations 'Kremsmuenster', 'Okehampton', 'Piacenza', 'Porto', 'Sevilla' and 'Thiva' by a double click on the location name in the left column. The result is shown in Figure 3.3. Then click on the 'Next' button.
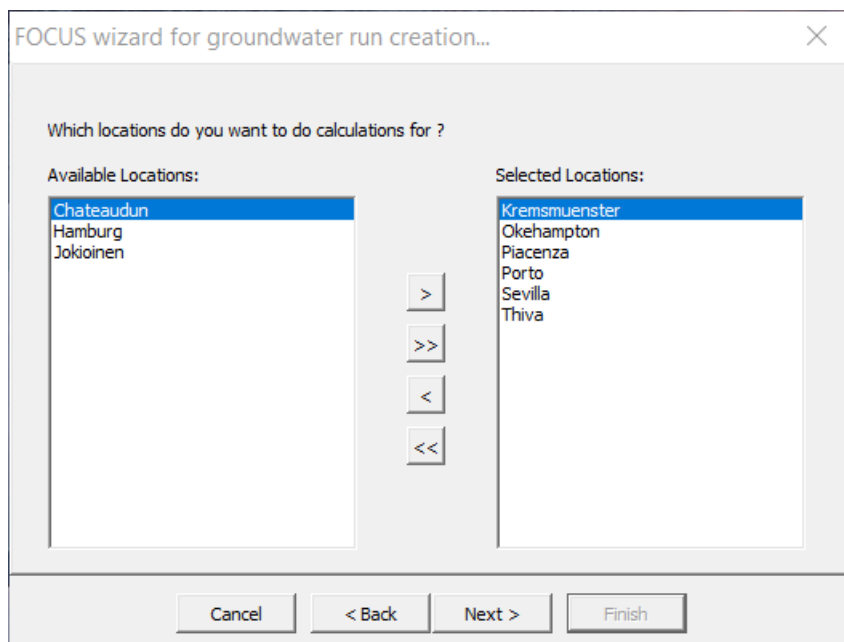
Figure 3.3 *The Groundwater wizard; the selection of locations.*

Step 5: Select the substance, the application scheme and the repeat interval.

The repeat interval can be 1, 2 or 3 for annual, biennial or triennial applications, respectively. The result is shown in Figure 3.4. It should be noted that only one of the existing substances or applications schemes can be selected. After completion click on the 'Next' button.
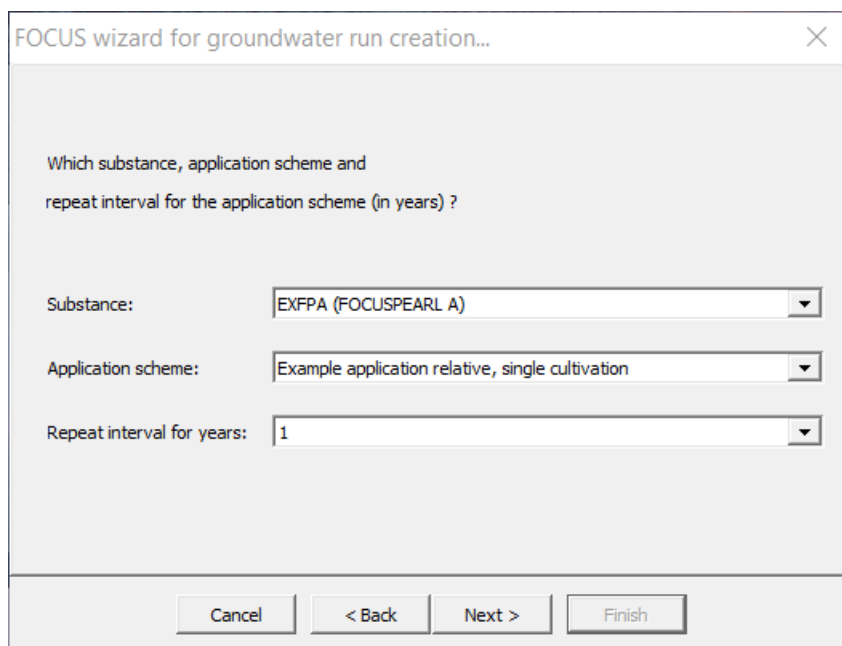
Figure 3.4 *The Groundwater wizard; the selection of the substance and its application scheme.*

Step 6: Create a new project or select an existing project to which the runs to be created are going to be assigned to. For this example a new project will be created. The resulting screen is shown in Figure 3.5.
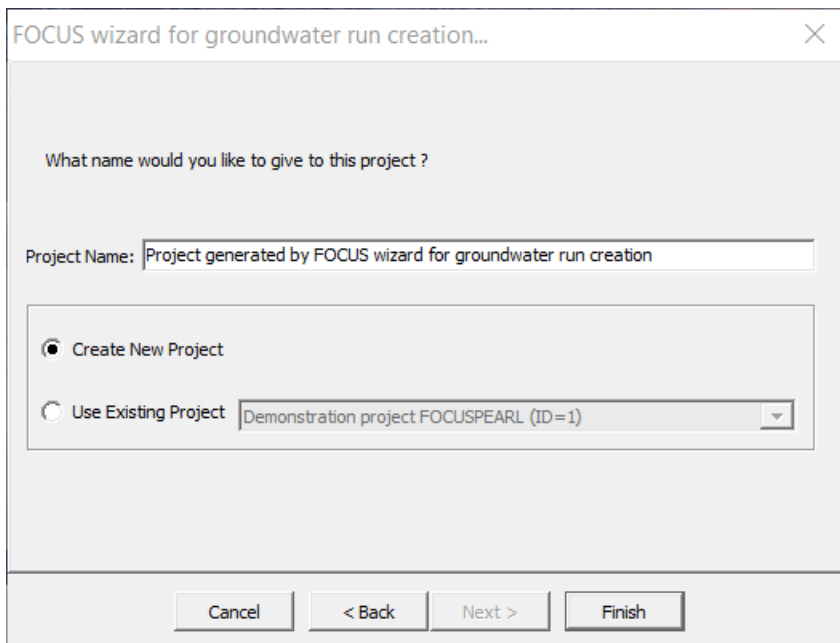
Figure 3.5   *The Groundwater wizard; the selection or creation of the project and its name.*

Then click on 'Finish'. The user interface starts retrieving the data for the scenario, the substance(s) and the application scheme. For this example 19 runs are created. It should be noted that most of the crops do not occur at every location.
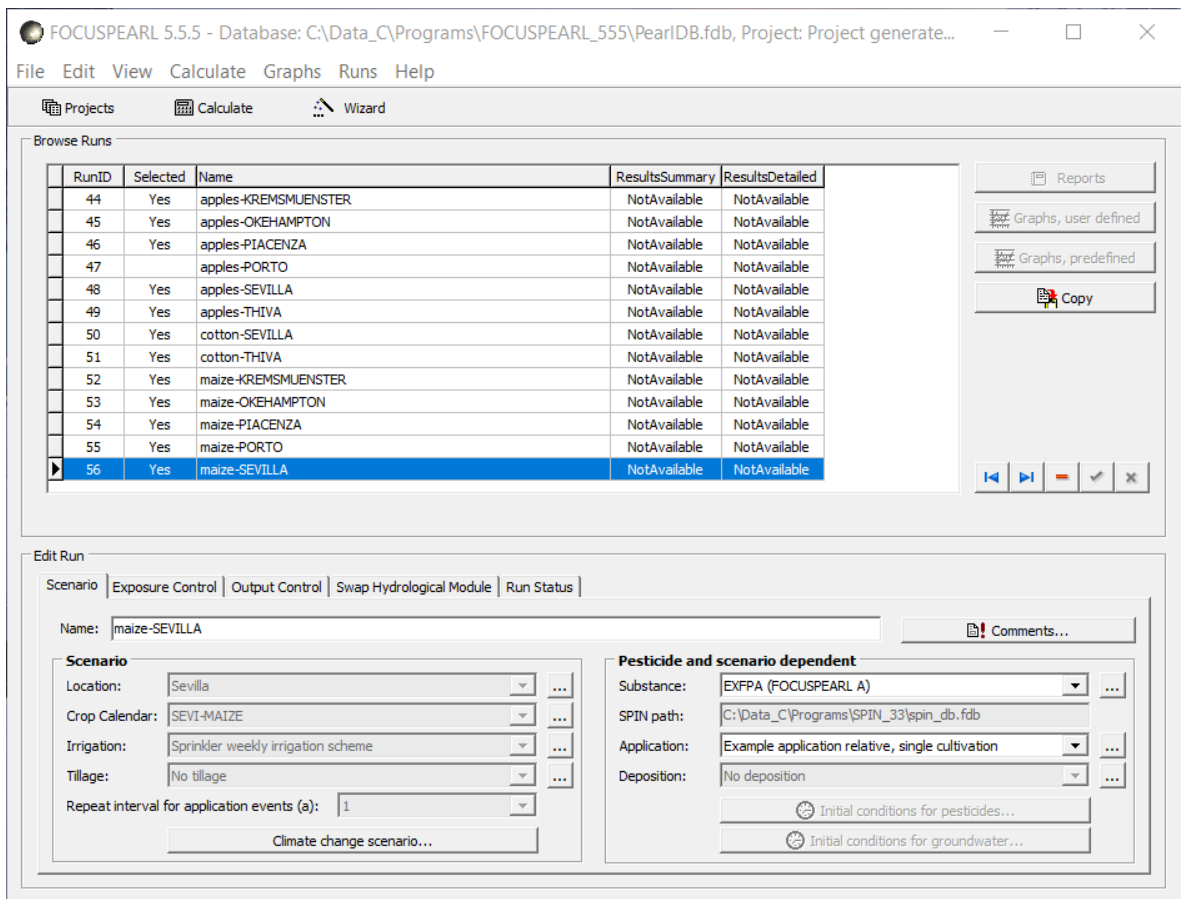
Figure 3.6   *The Groundwater wizard; the runs created by the Wizard.*

From the screen presented in Figure 3.6 most of the runs specifications are fixed and they cannot be changed. This is not the case for the substance and the application scheme. The user can change the substance and its application scheme for a particular run.

3.2 Running the model
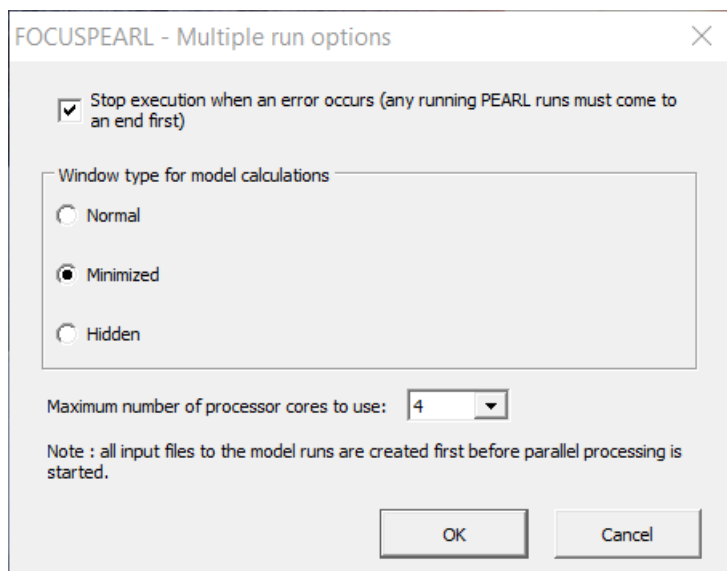
After the creation of the runs using the Wizard, the user can start the calculations by clicking on the button 'Calculate'. Next, the screen with input for multiple run options is shown (Figure 3.7).

In the upper part a checkbox is listed that gives the user the option to stop execution the moment an error occurs. Furthermore, there are three options available to the user for the window type for the model calculations:

- Normal; a window will pop up for each run to show the progress of the run.
- Minimized: all windows are put on the taskbar on the bottom of the screen. After clicking on one of the model run windows on the task bar, it will be presented on the screen of the computer, which allows the user to check the progress,
- Hidden: all model runs are executed on the background.

Using the 'Hidden' option, monitoring of the progress of the model runs is not possible. Only after all runs have been completed or if an error has occurred and the user has selected the checkbox 'Stop execution …' then the user gets back the control of the user interface.

In the lower section of the form the maximum number of cores that can be used to execute the model runs is listed. This maximum is equal to the total number of cores of the machine minus one. So one core is always available for other tasks on the machine.

Figure 3.7 *The form with the multiple run options.*

After all runs selected for execution have been run successfully, the user can view the results of each run. The availability status of the results for the runs in the project is shown in the columns "ResultsSummary" and "ResultsDetailed" (see Figure 3.6). By default the switch for a detailed output file is turned off, so only the summary results will be available.

It is possible to generate only the input files for the runs created by the Wizard. To do this the user has to select the option 'Create only input files' in the Calculate Menu as available at the top of the main screen. After this option has been selected, clicking on the 'Calculate' button only starts the generation of the input files. To execute the runs, the user has to select the option 'Calculate selected runs' in the Calculate menu.

3.3 Viewing the results

On the right-hand side of the main screen the button 'Graphs predefined' gives access to a form from which the user can select one of the standard graph types (see section 2.10.1). These are shown in Figure 3.8.
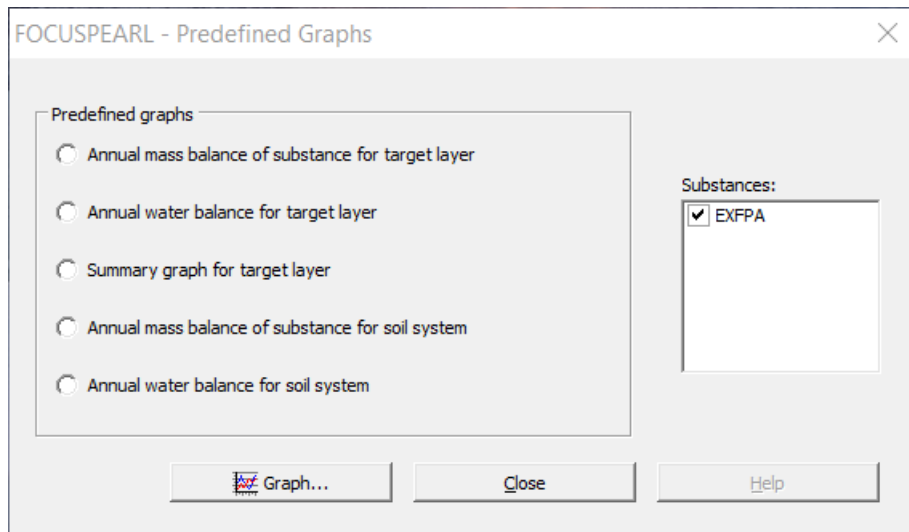
Figure 3.8 *The Predefined Graphs Form - the form to select one of the standard graph types.*

An example of one of these graphs, i.e. the Summary graph for the target layer is presented in Figure 3.9. The upper graph shows the frequency distribution of the leaching concentration at the target depth. For the FOCUS groundwater scenarios the target depth is 1 m and the target concentration is the 80th percentile of the leaching concentration at the target depth. For the use of example substance A for Apples in Kremsmuenster the target concentration is calculated to be 7.46 µg L^{-1}. This concentration is the average of the annual leaching concentration calculated for the simulation years 1913 and 1914 (indicated by arrows in the graph about the leaching concentrations calculated for the evaluation period. The lower two graphs show the mass leached from the FOCUS layer and the water percolated from this layer for the whole of the evaluation period.

Examples for the other two predefined graphs, i.e. the water balance and the mass balance are shown in Figures 3.10 and 3.11, respectively. Note that in the years 1922 and 1923 there is no water percolating below 1 m, so in these years the leaching concentration is equal to zero.
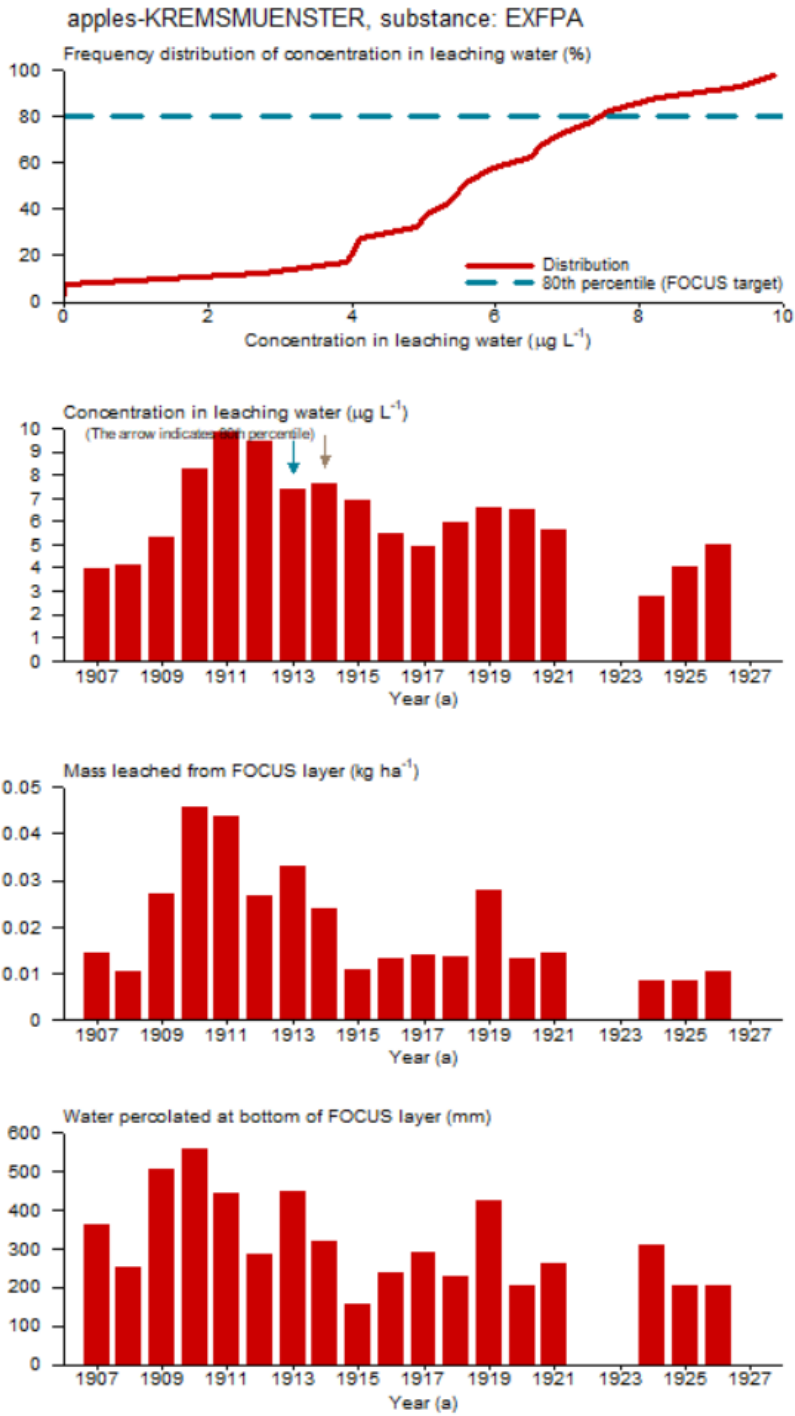
Figure 3.9: *Example of a FOCUS Summary graph*

apples-KREMSMUENSTER, substance: EXFPA
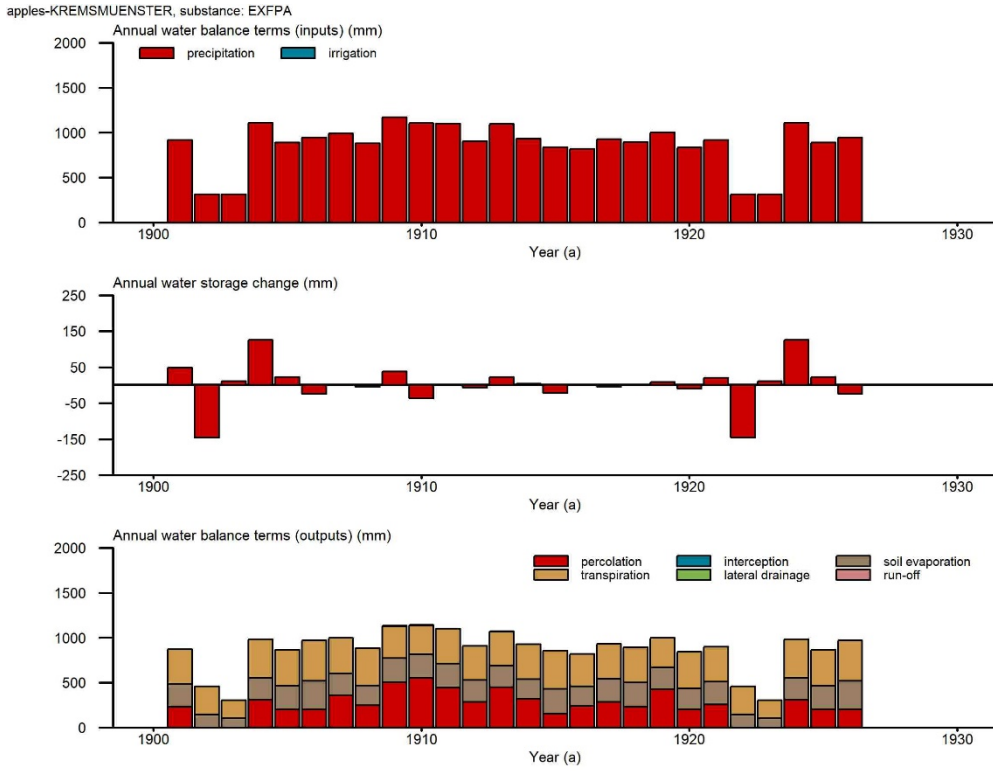
Figure 3.10 *Predefined graph: the water balance for the FOCUS target layer (1 m).*

apples-KREMSMUENSTER, substance: EXFPA
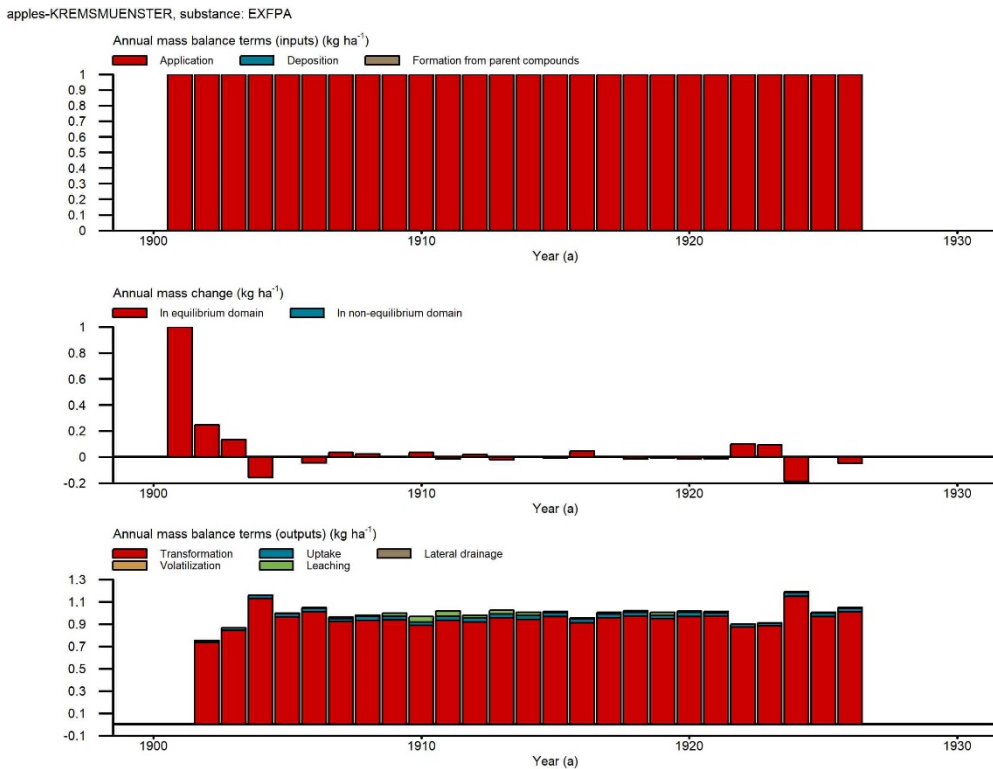
Figure 3.11 *Predefined graph: the mass balance for the FOCUS target layer (1 m).*

Reports on the results of the runs in the project can be generated by clicking on the Report button. Two report options are available (see Figure 3.12): one for the selected run only and one for the target results for all the runs in the project. An example report for a single run, i.e. for substance A for Apples in Kremsmuenster, is shown in Figure 3.13.
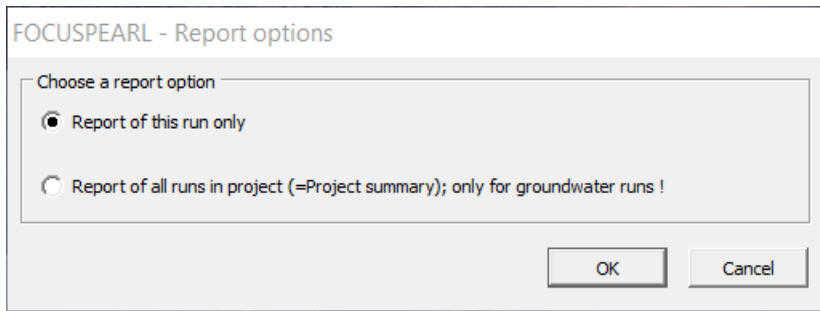
Figure 3.12 *Report options for groundwater runs .*

A report on all the runs in the project only presents the target concentration for the substances (including metabolites) for each run. This report can be shown in an Internet Browser or it can be copied to the clipboard.

```
* PEARL REPORT: Header
* Results from the PEARL model  (c) WENR, PBL and RIVM
* PEARL kernel version      : 3.2.16
* SWAP kernel version       : swap3237
* PEARL created on          : 19-Jul-2019
*
* PEARL was called from     : FOCUSPEARL,version 5.5.5
* Working directory         : C:\Data_C\Programs\FOCUSPEARL_555\PearlDB\44
* Run ID                    : 44
* Input file generated on   : 04-12-2019
* ------------------------------------------------------------------------------
*
* ExposureType        : Groundwater
* Location            : KREMSMUENSTER
* Meteo station       : krem-m
* Soil type           : KREM-S_Soil
* Crop calendar       : KREM-APPLES
* Substance           : EXFPA
* Application scheme   : EXAMPLE_RELATIVE_1_CULT
* Deposition scheme    : No
* Irrigation scheme    : No
*
* End of PEARL REPORT: Header

* PEARL REPORT: Leaching
* Start date    :    01-Jan-1901
* End date      :    31-Dec-1926
* Target depth  :    1.00 m
* Annual application to the soil surface at 31-Dec; dosage =     1.0000 kg.ha-1

* Leaching summary for compound EXFPA
* Molar mass (g.mol-1)                               :     300.0
* Saturated vapour pressure (Pa)                     :   0.100E-09; measured at (C)  20.0
* Solubility in water (mg.L-1)                       :    90.0    ; measured at (C)  20.0
* Half-life (d) in soil                              :      60.0; measured at (C)  20.0
* Kom (coef. for sorption on soil organic matter) (L.kg-1) :     60.0
* KF    (overall sorption coefficient of the soil target layer) (L.kg-1) :     0.918
* Freundlich exponent (-)                            :      0.90
* Plant uptake factor (-)                            :      0.50
* ----------------------------------------------------------------------------------------------------------------
* Period       From         To             Water percolated         Substance leached        Average substance
* number                                  below target depth (mm)   below target depth (kg/ha)  concentration in water
*                                                                                              at target depth (ug/L)
* ----------------------------------------------------------------------------------------------------------------
    1    01-Jan-1907 31-Dec-1907              362.626                0.0143016                    3.944
    2    01-Jan-1908 31-Dec-1908              250.082                0.0102621                    4.103
    3    01-Jan-1909 31-Dec-1909              505.425                0.0270322                    5.348
    4    01-Jan-1910 31-Dec-1910              554.086                0.0456736                    8.243
    5    01-Jan-1911 31-Dec-1911              442.959                0.0437598                    9.879
    6    01-Jan-1912 31-Dec-1912              283.112                0.0266329                    9.407
    7    01-Jan-1913 31-Dec-1913              448.114                0.0328837                    7.338
    8    01-Jan-1914 31-Dec-1914              315.868                0.0239411                    7.579
    9    01-Jan-1915 31-Dec-1915              154.478                0.0107128                    6.935
   10    01-Jan-1916 31-Dec-1916              237.736                0.0130354                    5.483
   11    01-Jan-1917 31-Dec-1917              286.443                0.0140809                    4.916
   12    01-Jan-1918 31-Dec-1918              228.576                0.0136514                    5.972
   13    01-Jan-1919 31-Dec-1919              423.996                0.0280335                    6.612
   14    01-Jan-1920 31-Dec-1920              201.883                0.0131266                    6.502
   15    01-Jan-1921 31-Dec-1921              258.099                0.0145066                    5.621
   16    01-Jan-1922 31-Dec-1922              -28.432               -0.0020329                    0.000
   17    01-Jan-1923 31-Dec-1923              -69.353               -0.0039834                    0.000
   18    01-Jan-1924 31-Dec-1924              307.212                0.0084154                    2.739
   19    01-Jan-1925 31-Dec-1925              202.904                0.0081642                    4.024
   20    01-Jan-1926 31-Dec-1926              202.555                0.0101906                    5.031

* The average concentration of EXFPA closest to the 80th percentile is      7.458856 ug/L
* End of PEARL REPORT: Leaching
```

Figure 3.13   *Example of a FOCUSPEARL Report for a groundwater assessment*

4 Using FOCUSPEARL for the EFSA PEC-soil scenarios

For the assessment of the exposure of organisms in the soil, guidance has been developed (EFSA, 2017). This guidance describes the evaluation procedure at the different tiers. For the assessments in the first two tiers the PERSAM model has been developed (EFSA, 2017). If the evaluation has to be continued at tier 3, then numerical models have to be used to calculate the exposure at specific sites. The main input data for these tier 3B assessments are generated by PERSAM. The input data are substance specific and they depend on the crop, the EU registration zone, the exposure concentration type, e.g. total content in soil or the concentration in pore water and the application method. Other input data are related to the site for which the tier 3B evaluation has to be done, e.g. the organic matter content in the topsoil and scaling factors for precipitation and temperature. The identification of these sites depends also on the coefficient of sorption to organic matter and the DT50 of the substance. Therefore, the evaluation sites for the parent substance will be different from those for the relevant metabolites. The PERSAM model generates a PERSAM transfer file (ptf) for each substance – exposure type – crop – zone combination.

The new version of FOCUSPEARL 5.5.5 facilitates the assessment of the soil exposure at tier 3B based on the ptf files as generated by PERSAM. The current version of PERSAM that needs to be used in combination with FOCUSPEARL 5.5.5 is PERSAM version 3.0. This version can be downloaded from the FOCUS DG SANTE Version Control website. This version should be installed in order to do the soil exposure assessments at tier 3B. An example of a ptf file is presented in Annex 3.

4.1 The Wizard for the creation of soil exposure assessments in FOCUSPEARL

After starting FOCUSPEARL, the main screen of the interface is shown. Just below the menu bar three buttons are shown, the 'Projects', 'Calculate' and 'Wizard' buttons. To generate soil exposure runs, the following procedure has to be followed.

Step 1: Start the FOCUSPEARL wizard by clicking on the 'Wizard' button. A window appears which gives two options for the wizard, which is shown in Figure 4.1.
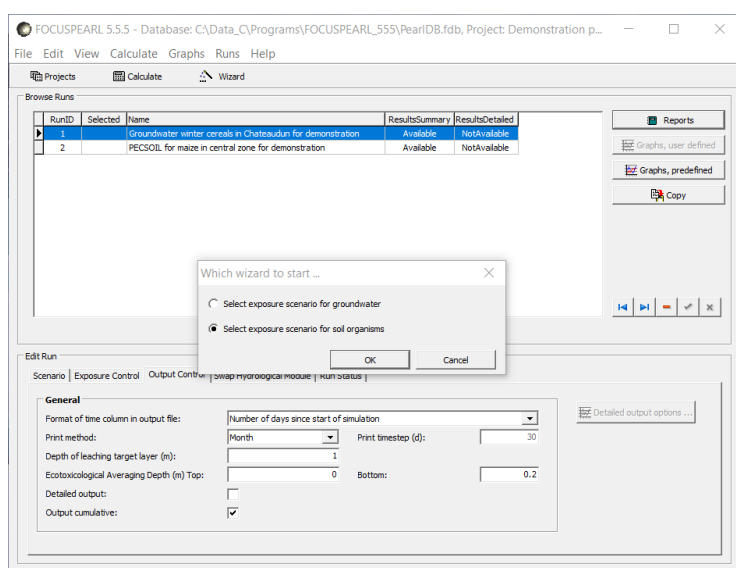
Figure 4.1   *The form to specify the type of Wizard: groundwater or soil exposure.*

Step 2: Select exposure scenario for soil organisms and click on the OK button. Next a window appears on the screen to navigate to the folder containing the ptf files created by PERSAM (see Figure 4.2). Then select the ptf files to be imported and click on the 'Open' button. After clicking the 'Open' button the form presented in Figure 4.3 is shown.
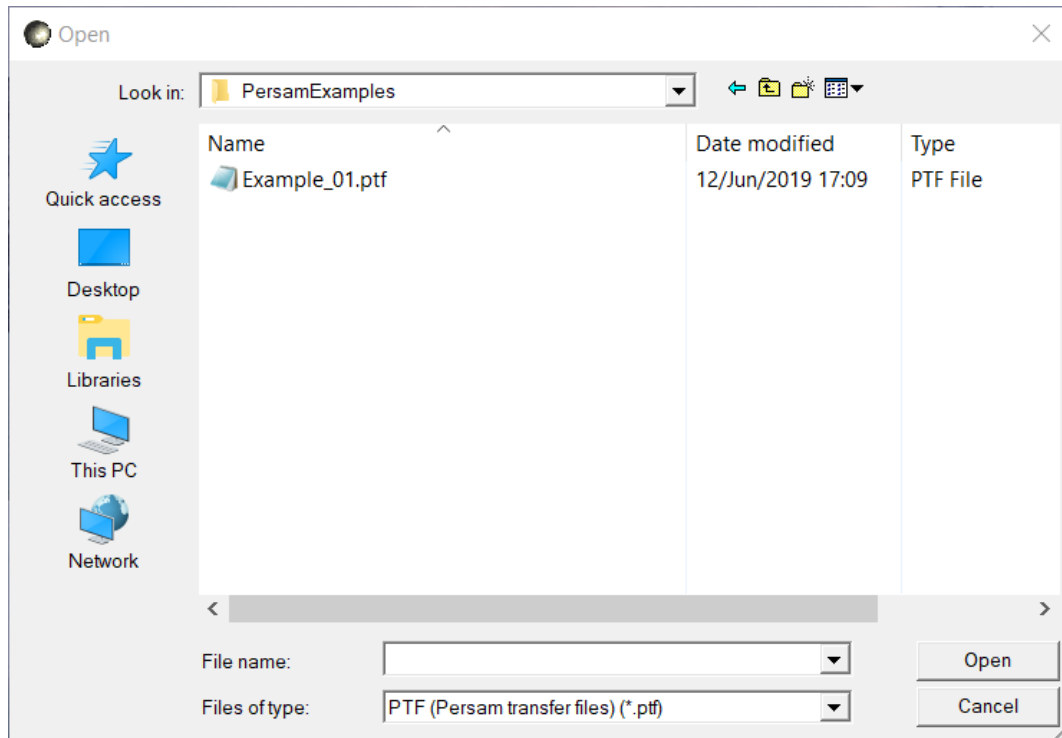
Figure 4.2: *The window to navigate and select the PERSAM transfer files.*

Step 3: Add other files by clicking on the button 'Add'. Then the 'Open' window as shown in Figure 4.2 appears. After all ptf files have been selected click on the 'Next' button. Then the application type form appears as presented in Figure 4.4.
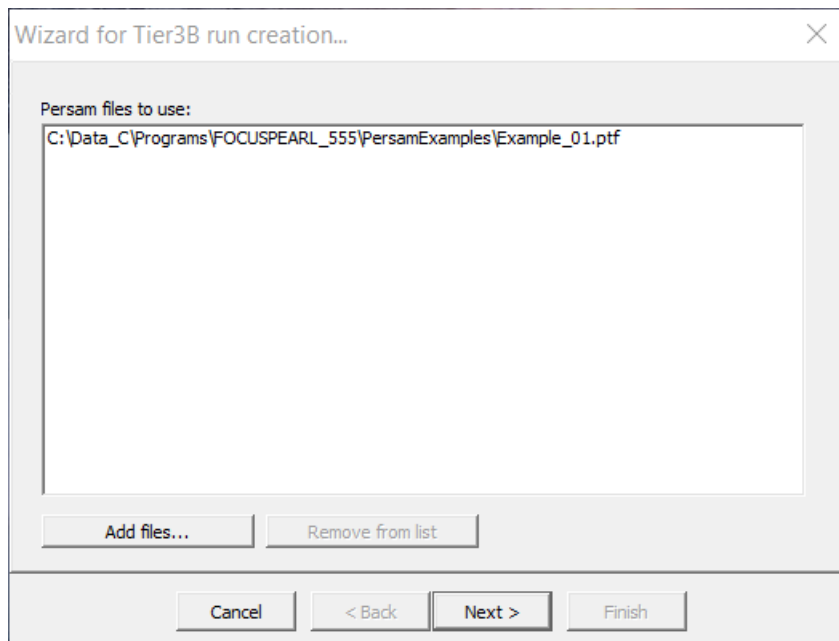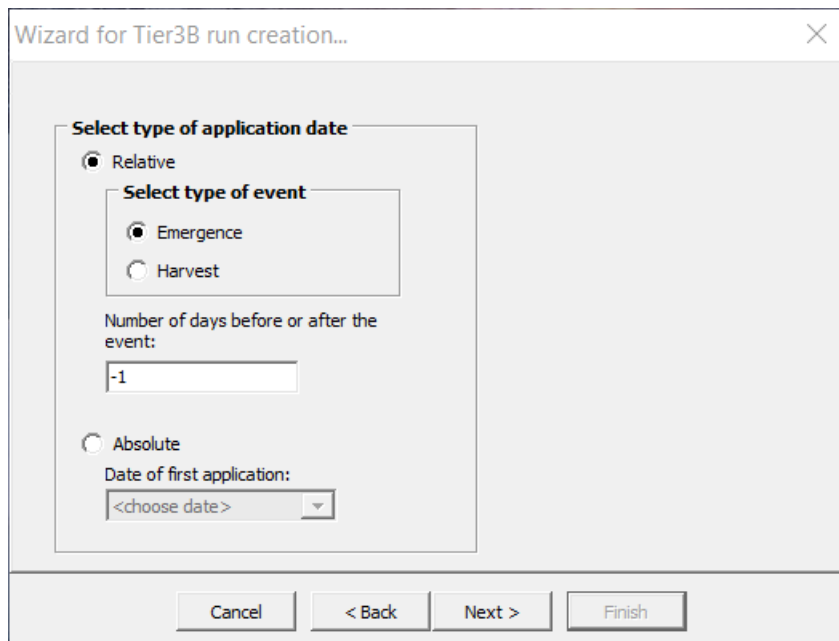
Figure 4.3   *The form showing the list of PERSAM transfer files to be imported.*
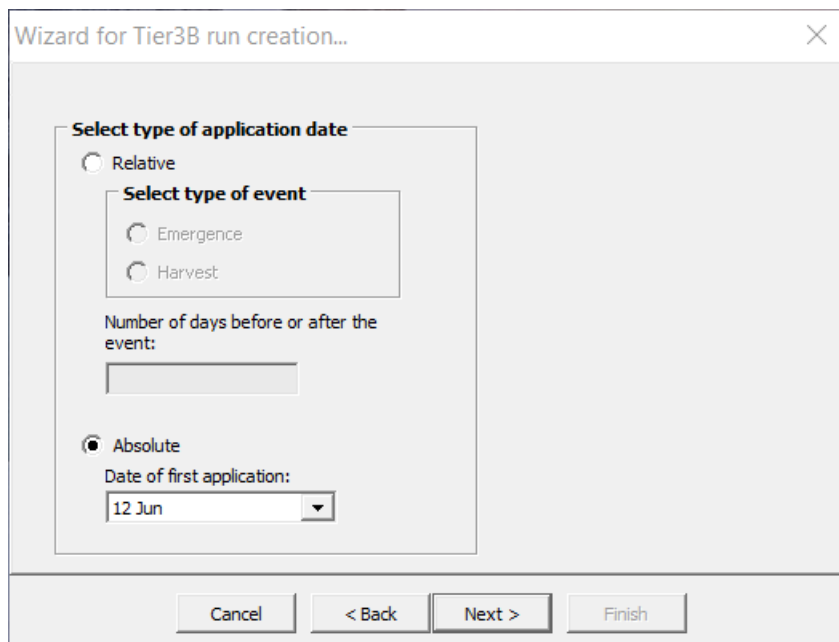
Step 4: Select the application scheme type and specify the first day of the application scheme.

As shown in Figure 4.4 two options are available: 'Absolute' and 'Relative'. In the form shown the option 'Relative' has been selected. The relative application date can be relative to the emergence of the crop or the crop harvest. To complete the data required for this application type, the number of days before or after the event need to be specified. A negative value implies an application before the crop event.

Figure 4.4   The application form to specify the application date type: relative to emergence.

If the user has selected the option 'Absolute', then the user has to enter the date of the first application. An example for the use of this option is shown in Figure 4.5. After completion of this form click on the 'Next' button.

Figure 4.5   The application form to specify the application date type: Absolute – Day and Month.

It should be noted that the application method as well as the rate of application are imported from the PERSAM ptf file. In this file the day number of the first application is always set to zero and if the application scheme contains more applications, then the number of days after the first application is given for this application in the ptf file.

Step 5: Create a new project or select an existing project to which the runs to be created are going to be assigned to. For this example a new project will be created. The resulting screen is shown in Figure 4.6.
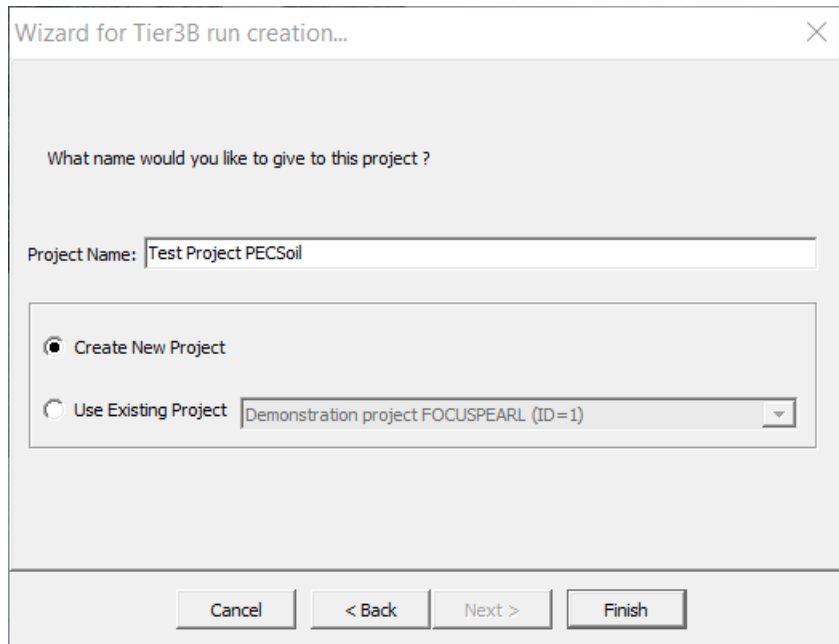
Figure 4.6 *The Groundwater wizard; the selection or creation of the project and its name.*

Then click on 'Finish'. The user interface starts retrieving the data for the scenario, the substance(s) and the application scheme. In this example only one run is generated as only the example ptf file has been selected. The user interface returns to the main screen showing the new project and the run in this project (see Figure 4.7).
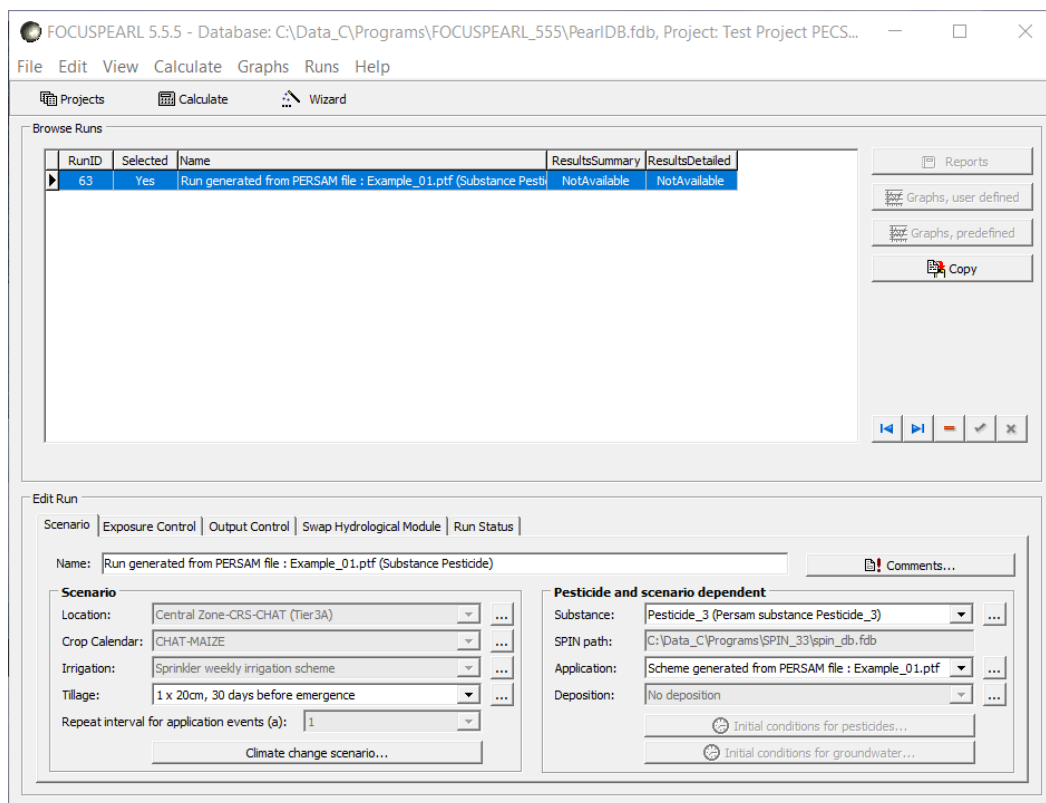
Figure 4.7 *The Soil Exposure wizard; the run created by the Wizard.*

Based on the information in the PERSAM ptf files, the following actions are executed by the user interface:

- A new parent substance and if present the metabolites of this compound are created in SPIN.
- An application scheme is created as selected in the wizard with the application method and application rates as specified in the ptf file
- All elements needed to complete the run characteristics: tillage scheme if relevant, FOCUS crop type, irrigation scheme if relevant and the location.

At the bottom of the screen a button 'Climate change scenario' is available to show the scaling factors for temperature and rainfall as specified in the ptf file. It should be noted that the name of the substance as specified in the ptf file is included in the name for this substance in SPIN. As each substance in SPIN must be unique, a number is added to the name of the substance as specified in the ptf. Moreover the name of the ptf file is also included in the description of the run and that of the application scheme.

4.2 Running the model

After the creation of the runs using the Wizard, the user can start the calculations by clicking on the button 'Calculate'. Next the screen with input for multiple run options is shown. These options have been explained in section 3.1 (See Figure 3.7).

Upon the successful completion of the runs in the project, the user can view the results of each run. The availability status of the results for the runs in the project is shown in the columns "ResultsSummary" and "ResultsDetailed" (see Figure 4.7). By default the switch for a detailed output file is turned off, so only the summary results will be available.

It is possible to generate only the input files for the runs created by the Wizard. To do this the user has to select the option 'Create only input files' in the Calculate Menu as available at the top of the main screen. After this option has been selected, clicking on the 'Calculate' button only starts the generation of the input files. To execute the runs, the user has to select the option 'Calculate selected runs' in the Calculate menu.

4.3 Viewing the results

On the right-hand side of the main screen the button 'Graphs predefined' gives access to a form from which the user can select one of the standard graph types (see section 2.10.1). These are shown in Figure 4.8.
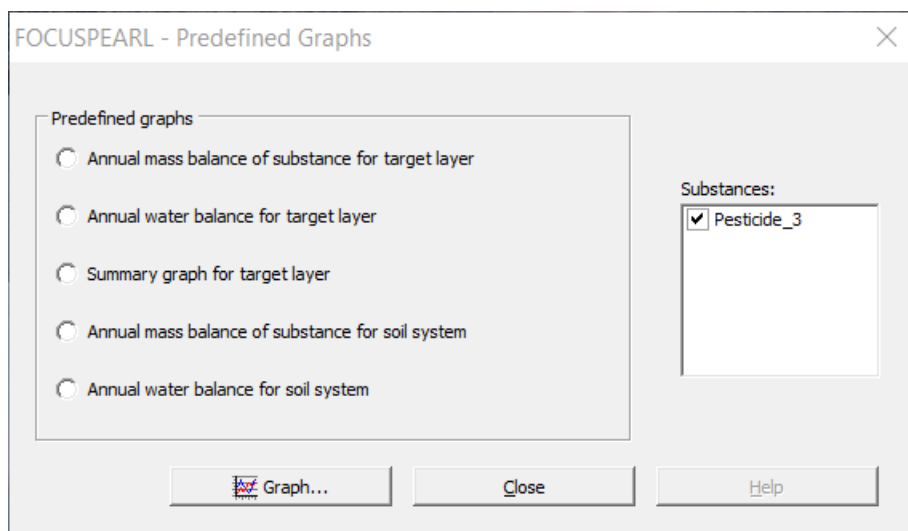
Figure 4.8   *The Predefined Graphs Form - the form to select one of the standard graph types.*

An example of one of these graphs, i.e. the Summary graph for the target layer is presented in Figure 4.9. It should be noted that the substance selected for this example has a DT50 in soil of 730 d and a coefficient for the sorption to organic matter of 1000 L kg^{-1}.
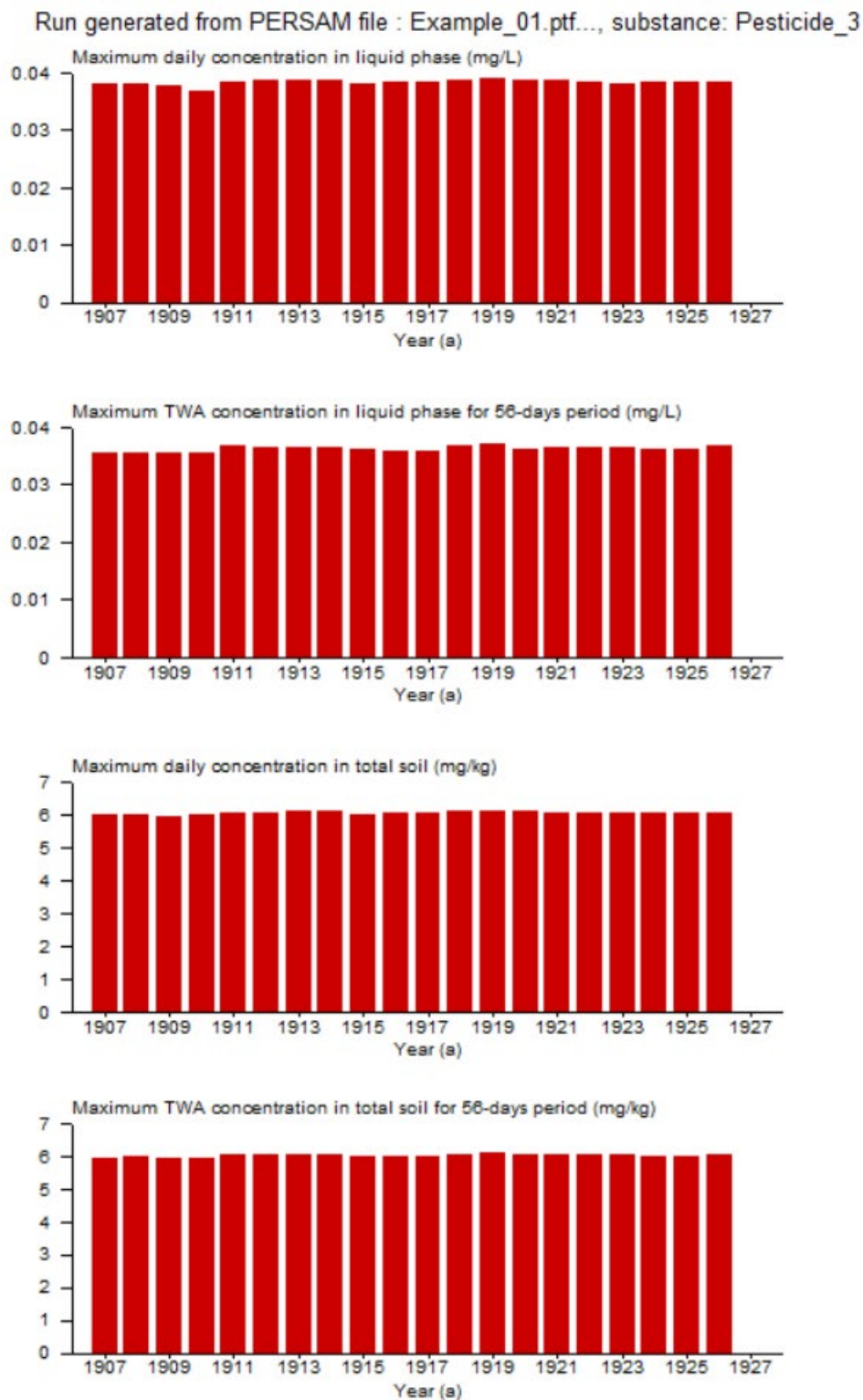
Figure 4.9: *Example of a Summary graph for the PEC Soil.*

Reports on the results of the runs in the project can be generated by clicking on the Report button (see Figure 3.12). For the soil exposure assessments only report option is available: the option for the selected run only. An example report for a single run, i.e. for substance example pesticide_3 for maize in the Central Zone is shown in Figure 4.10 and 4.11, for the first and second part of this report, respectively.

```
* PEARL REPORT: Header
* Results from the PEARL model  (c) WENR, PBL and RIVM
* PEARL kernel version      : 3.2.16
* SWAP kernel version       : swap3237
* PEARL created on          : 19-Jul-2019
*
* PEARL was called from     : FOCUSPEARL,version 5.5.5
* Working directory         : C:\Data_C\Programs\FOCUSPEARL_555\PearlDB\63
* Run ID                    : 63
* Input file generated on   : 05-12-2019
* ------------------------------------------------------------------------
*
* ExposureType            : SoilExposure
* Location                : C_CHAT-PS-M_CRS_T3A
* Meteo station           : chat-ps-m
* Soil type               : CRS-S_Soil
* Crop calendar           : CHAT-MAIZE
* Substance               : Pesticide_3
* Assessment substance  : Pesticide
* Application scheme      : ApplicatonSchemeRun_63
* Deposition scheme       : No
* Irrigation scheme       : SPRINKLER_WEEKLY
*
* End of PEARL REPORT: Header


* PEARL REPORT: Soil
* ----------------------------------------------------------------------------------------------------------------------
*
* Start date    :   01-Jan-1901
* End date      :   31-Dec-1927
* Thickness of evaluation layer  0.05 (m)
*
* This assessement is only valid for substance: Pesticide
*
* Annual application to the soil surface at 30-Apr; dosage =     1.0000 kg.ha-1
*
* Summary for substance Pesticide_3
* Molar mass (g.mol-1)                                      :    300.0
* Saturated vapour pressure (Pa)                           :  0.100E-07; measured at (C)  20.0
* Solubility in water (mg.L-1)                             :  0.100    ; measured at (C)  20.0
* Half-life (d) in soil                                    :    730.0; measured at (C)  20.0
* Kom (coef. for sorption on soil organic matter) (L.kg-1) :   1000.0
* KF   (overall sorption coefficient of the soil target layer) (L.kg-1) :     69.5
* Freundlich exponent (-)                                  :      0.90
* Plant uptake factor (-)                                  :      0.00

* Pore water concentration (mg/L)
  Pesticide_3  TWA_ConLiq_0      0.038860 at 30-Apr-1919
  Pesticide_3  TWA_ConLiq_1      0.038860 at 30-Apr-1919
  Pesticide_3  TWA_ConLiq_2      0.038848 at 30-Apr-1919
  Pesticide_3  TWA_ConLiq_3      0.038837 at 30-Apr-1919
  Pesticide_3  TWA_ConLiq_4      0.038827 at 30-Apr-1919
  Pesticide_3  TWA_ConLiq_7      0.038803 at 30-Apr-1919
  Pesticide_3  TWA_ConLiq_14     0.038671 at 30-Apr-1919
  Pesticide_3  TWA_ConLiq_21     0.038295 at 30-Apr-1919
  Pesticide_3  TWA_ConLiq_28     0.038017 at 30-Apr-1919
  Pesticide_3  TWA_ConLiq_56     0.037238 at 30-Apr-1919
  Pesticide_3  TWA_ConLiq_100    0.036283 at 30-Apr-1919
```

Figure 4.10   *Example of a FOCUSPEARL Report for soil exposure assessment – first part.*

```
* Concentration in total soil (mg/kg)
  Pesticide_3  TWA_CntSys_0      6.144703 at 30-Apr-1919
  Pesticide_3  TWA_CntSys_1      6.144703 at 30-Apr-1919
  Pesticide_3  TWA_CntSys_2      6.143839 at 30-Apr-1919
  Pesticide_3  TWA_CntSys_3      6.143107 at 30-Apr-1919
  Pesticide_3  TWA_CntSys_4      6.142552 at 30-Apr-1919
  Pesticide_3  TWA_CntSys_7      6.141174 at 30-Apr-1919
  Pesticide_3  TWA_CntSys_14     6.137644 at 30-Apr-1919
  Pesticide_3  TWA_CntSys_21     6.132588 at 30-Apr-1919
  Pesticide_3  TWA_CntSys_28     6.127095 at 30-Apr-1919
  Pesticide_3  TWA_CntSys_56     6.095048 at 30-Apr-1919
  Pesticide_3  TWA_CntSys_100    6.015645 at 30-Apr-1919

* Yearly maximum total content in soil and date of occurrence (mg/kg)
 1907  Pesticide_3    5.998213  TWA_CntSys_0   30-Apr-1907
 1908  Pesticide_3    6.026991  TWA_CntSys_0   30-Apr-1908
 1909  Pesticide_3    5.974360  TWA_CntSys_0   30-Apr-1909
 .
 .
 .
 1924  Pesticide_3    6.082540  TWA_CntSys_0   30-Apr-1924
 1925  Pesticide_3    6.065556  TWA_CntSys_0   30-Apr-1925
 1926  Pesticide_3    6.084343  TWA_CntSys_0   30-Apr-1926

* Yearly maximum TWA 56 d pore water concentration and date of occurrence (mg/L)
 1907  Pesticide_3    0.035612  TWA_ConLiq_56  30-Apr-1907
 1908  Pesticide_3    0.035555  TWA_ConLiq_56  30-Apr-1908
 1909  Pesticide_3    0.035426  TWA_ConLiq_56  30-Apr-1909
 .
 .
 .
 1924  Pesticide_3    0.036178  TWA_ConLiq_56  30-Apr-1924
 1925  Pesticide_3    0.036132  TWA_ConLiq_56  30-Apr-1925
 1926  Pesticide_3    0.036830  TWA_ConLiq_56  30-Apr-1926

* Yearly maximum TWA 56 d total content in soil and date of occurrence (mg/kg)
 1907  Pesticide_3    5.927517  TWA_CntSys_56  30-Apr-1907
 1908  Pesticide_3    5.976362  TWA_CntSys_56  30-Apr-1908
 1909  Pesticide_3    5.903020  TWA_CntSys_56  30-Apr-1909
 .
 .
 .
 1924  Pesticide_3    6.012292  TWA_CntSys_56  30-Apr-1924
 1925  Pesticide_3    5.997096  TWA_CntSys_56  30-Apr-1925
 1926  Pesticide_3    6.026791  TWA_CntSys_56  30-Apr-1926
*
* The value for the refinement factor for final PEC as specified by PERSAM is:   1.000
* A value for PERSAM_fRef less than 1.00 implies a non-uniform application
* All pore water concentrations and total contents in soil in this summary have been multiplied by this factor
*
* The quantities reported in the following lines are averages over the top 20 cm of soil.
*
* Average pore water concentration of substance Pesticide_3 at 200 days after last application:   0.031122 mg/L
* Average total content in soil of substance Pesticide_3 at 200 days after last application:      5.359551 mg/kg
*
* The following two lines gives the results on the plateau concentrations
* Pore water plateau concentration of substance Pesticide_3:    0.022425 mg/L ; plateau reached just before the application on 30-Apr-1919
* Plateau of total content in soil of substance Pesticide_3:    4.003290 mg/kg; plateau reached just before the application on 30-Apr-1919

* End of PEARL REPORT: Soil
```

Figure 4.11   *Example of a FOCUSPEARL Report for soil exposure assessment – second part.*

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Justification

Annex 1 The FOCUSPEARL_555 PEARL input file

```
* Section 0: Run identification and model version
* Section 1: Control section
* Section 2: Soil section
* Section 3: Weather and irrigation data
* Section 4: Boundary and initial conditions of hydrological model
* Section 5: Compound section
* Section 6: Management section
* Section 7: Initial and boundary conditions of pesticide fate model
* Section 8: Crop section
* Section 9: Output control


*-------------------------------------------------------------------------------------
* Section 0: Run identification
*-------------------------------------------------------------------------------------

Groundwater            ExposureType         Scenario identification
Hamburg                Location             Location identification
HAMB-S_Soil            SoilTypeID           Soil identification
HAMB-SUGARBEET         CropCalendar         Crop calendar
pest                   SubstanceName        Substance name
ExampleScheme          ApplicationScheme    Application scheme
No                     DepositionScheme     Deposition scheme
No                     IrrigationScheme     Irrigation scheme

* if ExposureType set to 'SoilExposure' then AssessmentSubstance is reported
pest                   AssessmentSubstance   Name assessment substance


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

* Release type option CallingProgram
* Options can be: FOCUSPEARL, GEOPEARL, DRAINBOW, CHINAPEARL and GEM.

FOCUSPEARL             CallingProgram       Release type
5.5.5                  CallingProgramVersion Version numbers of model, interface and database
Groundwater            ExposureType         Options are: Groundwater, SoilExposure, Other

* If ExposureType set to 'SoilExposure' then specify ExposureEndPoint and PERSAMLocation
PoreWat                ExposureEndPoint     Options are PoreWat and TotSol
5414000_1890000        PERSAMLocation       PERSAM XY-coordinates of pixel selected

* Time domain
01-Jan-1901            TimStart             Begin time of simulation [01-Jan-1900|-]
31-Dec-1926            TimEnd               End time of simulation [TimStart|-]

* Specify warming-up period
6                      InitYears (y)        Length of warming-up period
0                      NumRep (-)           Number of times warming-up period is repeated
* NumRep only required for ExposureType 'SoilExposure'

* SWAP control
* Options to run SWAP using OptHyd
* OnLine         Runs SWAP and then PEARL
* OffLine        Assumes a pfo file with hydrological output from SWAP
* Automatic      Skip SWAP if SWAP run has already been done
* Only           Run SWAP only and process results in PEARL output format
* Standard       Select the .pfo as specified by the user
* GenerateInput  Generate the input files for SWAP
OnLine                 OptHyd               Option selected to run SWAP
* If OptHyd is 'Standard' then specify SWAPId to identify SWAP pfo file
Summer                 SwapID               Dutch surface water standard scenario for
summer
                                            crops
1.d-5                  DelTimSwaMin (d)     Minimum time step in SWAP [1d-8|0.1]
0.1                    DelTimSwaMax (d)     Maximum time step in SWAP [0.01|0.5]
0.001                  ThetaTol     (m3.m-3) Tolerance in SWAP [1e-5|0.01]
9.9                    GWLTol       (m)     Tolerance for groundwater level
30                     MaxItSwa             Maximum number of iterations in SWAP [1|100]

* If OptMacropore set to 'Yes' then specify additional input parameters
0.00001                DelTimMinPrl (d)     Minimum time-step in PEARL
```

* Option to specify output interval. The options are: Hour, Day, Decade Month, Year,
Automatic * or Other
* If automatic then output interval calculated - always 1000 steps
Day   OptDelTimPrn   Option to set output interval

* If Other then specify time interval
30   DelTimPrn   (d)   Print time step [1|-]
End if

Yes   OptScreen   Option to write output to screen

*
All   OptSys   Option to define system: All (plant and soil)
or
                                 PlantOnly
* If PlantOnly then soil profile data are not needed, except SoilTypeID and Location

No   OptPaddy   Option to assess paddy rice system: Yes or No

None   OptAux   Option for auxiliary output

*--
* Section 2: Soil section
* Description
*--
* The soil profile
* Specify for each horizon:
* Horizon thickness (m)
* The number of soil compartments [1|500]
* Nodes are distributed evenly over each horizon

table SoilProfile
ThiHor NumLay
(m)
0.01   5
0.29   29
0.3   24
0.15   6
0.15   6
0.1   4
0.5   10
3   30
end_table

* Basic soil parameters
* Specify for each soil horizon:
* Mass content of sand, expressed as a fraction of the mineral soil (kg.kg-1) [0|1]
* Mass content of silt, expressed as a fraction of the mineral soil (kg.kg-1) [0|1]
* Mass content of clay, expressed as a fraction of the mineral soil (kg.kg-1) [0|1]
* Organic matter mass content   (kg.kg-1) [0|1]
* pH. pH measured in 0.01 M CaCl2 is preferred (see theory document) (-)   [1|13]
table horizon SoilProperties
Nr   FraSand   FraSilt   FraClay   CntOm   pH
      (kg.kg-1) (kg.kg-1) (kg.kg-1) (kg.kg-1)   (-)
1   0.683   0.245   0.072   0.026   6.4
2   0.683   0.245   0.072   0.026   6.4
3   0.67   0.263   0.067   0.017   5.6
4   0.962   0.029   0.009   0.0034   5.6
5   0.998   0.002   0   0   5.7
6   1   0   0   0   5.5
7   1   0   0   0   5.5
8   1   0   0   0   5.5
end_table

* Parameters of the Van Genuchten-Mualem relationships (B1 + O1)
* Specify for each soil horizon:
* The saturated water content   (m3.m-3) [0|0.95]
* The residual water content   (m3.m-3) [0|0.04]
* Parameter AlphaDry   (cm-1)   [1.d-3|1]
* Parameter AlphaWet   (cm-1)   [1.d-3|1]
* Parameter n   (-)   [1|5]
* The saturated conductivity   (m.d-1)   [1.d-4|10]
* Parameter lambda (l)   (-)   [-25|25]
* If OptMacropore 'Yes' then specify
* Entry pressure head PreHeaEnt   (cm)
* Anisotropy coefficient   (-)
* New Staring Series - not used for standard scenario

table horizon VanGenuchtenPar

```
Nr ThetaSat   ThetaRes   AlphaDry   AlphaWet    n      KSat      l
   (m3.m-3)   (m3.m-3)   (cm-1)     (cm-1)      (-)    (m.d-1)   (-)
1   0.391      0.036      0.0149     0.0298     1.468  2.016     0.5
2   0.391      0.036      0.0149     0.0298     1.468  2.016     0.5
3   0.37       0.03       0.0126     0.0252     1.565  2.736     0.5
4   0.351      0.029      0.0181     0.0362     1.598  2.448     0.5
5   0.31       0.015      0.0281     0.0562     1.606  2.448     0.5
6   0.31       0.015      0.0281     0.0562     1.606  2.448     0.5
7   0.31       0.015      0.0281     0.0562     1.606  2.448     0.5
8   0.31       0.015      0.0281     0.0562     1.606  2.448     0.5
end_table


Input           OptRho                          Option for bulk density: Calculate or Input
* If RhoOpt = Input then specify bulk density for each horizon:
table horizon    Rho             (kg.m-3)    [100|2000]
1   1500.0
2   1500.0
3   1600.0
4   1560.0
5   1620.0
6   1600.0
7   1600.0
8   1600.0
end_table
* End If


* If RhoOpt = Calculate then no extra data are needed on bulk density


* Option to include hysteresis
No              OptHysteresis                   Hysteresis option: No, InitWetting InitDrying


* If No or InitDrying then specify minimum pressure head
0.2             PreHeaWetDryMin (cm)            Minimum pressure head to switch drying/wetting


* Maximum ponding depth and boundary air layer thickness (both location properties)
0.01            ZPndMax         (m)             Maximum ponding depth [0|1]


* If OptMacropore is 'Yes' then specify boundary pressure head that controls run-off
0.0             Hb              (cm)            Boundary pressure head
0.001           RstSurRunOff    (d)             Resistance for surface runoff
* End if


* Soil evaporation parameters
1.2             FacEvpSol       (-)             "Crop factor" for bare soil [0.5|1.5]


* Option to select evaporation reduction method: Boesten or Black
Boesten         OptSolEvp                       Evaporation reduction option
* If Boesten or Black specify soil evaporation parameters

0.79            CofRedEvp       (cm1/2)         Parameter in Boesten equation [0|1]
0.01            PrcMinEvp       (m.d-1)         Minimum rainfall to reset reduction


* Parameter values of the functions describing the relative diffusion coefficients
MillingtonQuirk  OptCofDifRel                   MillingtonQuirk, Troeh or Currie


* If MillingtonQuirk:
2.0             ExpDifLiqMilNom (-)             Exponent in nominator of equation [0.1|5]
0.67            ExpDifLiqMilDen (-)             Exponent in denominator of eqn    [0.1|2]
2.0             ExpDifGasMilNom (-)             Exponent in nominator of equation [0.1|5]
0.67            ExpDifGasMilDen (-)             Exponent in denominator of eqn    [0.1|2]


* If Troeh:
0.05            CofDifLiqTro    (-)             Coefficient in Troeh equation      [0|1]
1.4             ExpDifLiqTro    (-)             Exponent in Troeh equation         [1|2]
0.05            CofDifGasTro    (-)             Coefficient in Troeh equation      [0|1]
1.4             ExpDifGasTro    (-)             Exponent in Troeh equation         [1|2]


* If Currie:
2.5             CofDifLiqCur    (-)             Coefficient in Currie equation     [0|-]
3.0             ExpDifLiqCur    (-)             Exponent in Currie equation        [1|-]
2.5             CofDifGasCur    (-)             Coefficient in Currie equation     [0|-]
3.0             ExpDifGasCur    (-)             Exponent in Currie equation        [1|-]


* End If


* Dispersion length of solute in liquid phase [0.5Delz|1]
Table horizon LenDisLiq (m)
1  0.05
2  0.05
3  0.05
```

```
4  0.05
5  0.05
6  0.05
7  0.05
8  0.05
end_table

* Ponding of water on soil surface: Constant or TimeDependent
Constant         OptPnd                      Option for ponding of water
* If TimeDependent specify file with data on ponding depth
FileId           PondingDepthFile


    *-------------------------------------------------------------------
    * Section 2a: Macropore section
    * Only required if OptMacropore set to 'Yes'
    *-------------------------------------------------------------------

No               OptMacropore                Simulate macropore flow (Yes|No)

    *---------------------------------------------------------------------------
    * Section 3: Weather and irrigation data
    * Description
    *---------------------------------------------------------------------------

hamb-m           MeteoStation                Maximum 7 characters.
Input            OptEvp                      Evapotranspiration: Input, Penman,
                                             PenmanMonteith or Makkink

* if ExposureType set to 'SoilExposure' then specify OptCov
LAI              OptCov                      Option to calculate interception: LAI or
*                                            CovSol (Soil Cover)

52.0             Lat                         Latitude of meteo station [-60|60]
10.0             Alt             (m)         Altitude of meteo station [-400|3000]

* Initial lower boundary soil temperature [-20|40]
* Upper boundary temperature is read from meteo file
12.6             TemLboSta       (C)

* Irrigation section
No               OptIrr
* Options for OptIrr are:
* No: no irrigation
* Surface: Surface irrigation, irrigation depth spec. by user
* Surface_Auto: Surface irrigation, irrigation depth calc. by model
* Sprinkler: Sprinkler irrigation, irrigation depth spec. by user
* Sprinkler_Auto: Sprinkler irrigation, irrigation depth calc. by model
* Sprinkler_Weekly: Sprinkler irrigation, irrigation depth calc. by user

FileName         IrrigationData              Name of file with irrigation data
* Irrigation data have to be provided in a file Station.irr (e.g. debilt.irr);
* Maximum number of characters in filename is 7.
* If RepeatHydrology is set to Yes, the first year is required only
* Format of the file should be as below:
* table IrrTab (mm)
* 01-Aug-1980 10.0
* end_table
1.0              FacPrc (-)                  Correction factor for precipitation
0.0              DifTem (C)                  Correction for temperature
1.0              FacEvp (-)                  Correction factor for evapotranspiration
Daily            OptMetInp                   Option for meteorological data: Hourly or
Daily

* Options for the calculation of the resistance of air to volatilisation; options are
Laminar
* or Aerodynamic
* If set to 'Aerodynamic' then OptResBou is also required: options are Hicks or Wang
* If set to 'laminar' then ThiAirBouLay required
Laminar          OptTraRes                   Option for resistance air set to Laminar
If set to 'Laminar' then specify thickness boundary air layer
0.01             ThiAirBouLay    (m)         Boundary air layer thickness [1e-6|1]
* If set to 'Aerodynamic' then OptResBou is also required: options are Hicks or Wang
Hicks            OptResBou       (-)         Option to calculate resistance boundary layer
0.01             LenRghMmtLcl    (m)         Specify local roughness length
10.0             ZMeaWnd         (m)         Specify measurement height for wind speed
* End if

No               OptRainfallEvents           Option to consider rainfall events
* If set to 'Yes' then specify duration of events
0.1              LenRainfall (d)
```

```
No              OptSnow                         Option to consider snow in SWAP
*-----------------------------------------------------------------------------------
* Section 4:  Boundary and initial conditions of hydrological model
* Section 4a: Lower boundary flux conditions
* Description
*-----------------------------------------------------------------------------------

* Initial condition
-200.0          ZGrwLevSta      (cm)            Initial groundwater level [-5000|0]

* Choose one of the following options for the bottom boundary:
* GrwLev Flux Cauchy FncGrwLev Dirichlet ZeroFlux FreeDrain Lysimeter
FncGrwLev       OptLbo                          Lower boundary option selected

* If LboOpt = GrwLev specify file with groundwater level data
* FileId          LowerBoundaryFile

* Read from LowerBoundaryFile (FileId.bot)
* table   GrwLev   (cm)                         Groundwater level [-|0]
* 01-Jan-1901  -100.0
* 31-Dec-1926  -100.0
* end_table
* End if

* If LboOpt = Flux then specify flux lower boundary option
* Options for bottom flux can be Sine or Table
* HeadOnly        OptbotFlux                    Option selected for bottom flux
* If OptbotFlux = Sine then specify average, amplitude and day of maximum
* -0.250          FlvLiqLboAvg    (m.a-1)       Average annual lower boundary flux [-1|1]
* 0.10            FlvLiqLboAmp    (m)           Amplitude of lower-boundary flux [0|0.5]
* 01-Oct          DayFlvLiqLboMax               Day of maximum flux [01-Jan|31-Dec]
* If OptbotFlux = Table then specify file with flux data
* FileId          LowerBoundaryFile
* End if

* If LboOpt = Cauchy then specify lower boundary option
* Options for bottom flux can be Sine, HeadOnly or HeadAndFlux
* HeadOnly        OptBotFlux                    Option selected for bottom flux
* No              OptNoResVert                  Switch on or switch off vertical resistance
* NoDrains        OptShapeGrwLev                Elliptic, Parabolic, Sinusoidal, NoDrains
* -0.8200         HeaDraBase      (m)           Drainage base to correct GrwLev [-100|0]
* 5.0             RstAqt          (d)           Resistance of aquitard [0|1e4]

* If OptBotFlux = Sine then specify average, amplitude and day of maximum
-1.4            HeaAqfAvg       (m)           Mean hydraulic head of aquifer [-10|10]
0.2             HeaAqfAmp       (m)           Amplitude of aquifer hydraulic head [0|10]
01-May          DayHeaAqfMax    (d)           Day with maximum head [01-Jan|31-Dec]

* If OptBotFlux HeadOnly or HeadAndFlux specify file with data
* Lower boundary conditions
BBW             LowerBoundaryFile
* If HeadOnly then read data on Head from LowerBoundaryFile (FileId.bot)
* table HeaAqfAve (cm)
* 01-Jan-1901  -100.0
* 31-Dec-1926  -100.0
* end_table
* End if

* If HeadAndFlux then read data on Head and Flux from LowerBoundaryFile (FileId.bot)
* table HeaAqfAve  QBot
* 01-Jan-1901  -100.0  0.003
* 31-Dec-1926  -100.0  0.005
* end_table
* End if

* If LboOpt = FncGrwLev (flux boundary condition - flux is a function of groundwater level)
-0.01           CofFncGrwLev    (m.d-1)       Coefficient in Q(h) relationship [-1|1]
-1.4            ExpFncGrwLev    (m-1)         Exponent in Q(h) relationship [-100|100]

* LboOpt = Dirichlet the read data on pressure head boundary condition from file FileId.bot
* FileId          LowerBoundaryFile
* table   h  (m)                              Pressure head [-1e4|1e4]
* 01-Jan  -1.0
* 31-Dec  -1.0
* end_table


*-----------------------------------------------------------------------------------
* Section 4b: Local drainage fluxes to ditches and drains
*-----------------------------------------------------------------------------------
No              OptDra                          No, Basic or extended drainage module
0               NumDraLev                       Number of drainage levels (0|5)
```

```
* If OptDra =\ No then NumDraLev cannot be zero.

No               OptSurDra                    Option to consider rapid subsurface drainage

*-----------------------------------------------------------------------------------
* Section 5: Compound section
* Description
*-----------------------------------------------------------------------------------

* Compounds. First compound is the parent pesticide, the others are metabolites.
table compounds
pest
end_table
200.0            MolMas_pest    (g.mol-1)    Molar mass [10|10000]

* Name assessment substance relevant for ExposureType option 'SoilExposure'. In that case
only the results of the assessment substance (parent or one of the metabolites) can be
reported for the exposure assessment.
pest                     AssessmentSubstance   Name assessment substance

* Transformation table (parent-daughter relationships)
*

table FraPrtDau (mol.mol-1)
end_table

* Example for a pesticide with three metabolites, named "met1", "met2" and "met3":
* Reaction 1: pest is transformed into met1 (25%)
* Reaction 2: pest is transformed into met2 (44%)
* Reaction 3: met1 is transformed into met3 (63%)
* table FraPrtDau (mol.mol-1)
* 0.25 pest -> met1
* 0.44 pest -> met2
* 0.63 met1 -> met3
* end_table

* Transformation rate parameters
EqlDom_Input     OptDT50_pest                 Option for DT50: Input or Calculate in
                                              equilibrium domain (EqlDom) or in liquid phase
                                              only (LiqPhs)
50.0             DT50Ref_pest   (d)           Half-life time [1|1e6]
20.0             TemRefTra_pest (C)           Temperature at which DT50 is measured [5|30]
0.70             ExpLiqTra_pest (-)           Exponent for the effect of liquid [0|5]
OptimumConditions OptCntLiqTraRef_pest        OptimumConditions or NonOptimumConditions
1.0              CntLiqTraRef_pest (kg.kg-1)  Liq. content at which DT50 is measured [0|1]
65.4             MolEntTra_pest (kJ.mol-1)    Molar activation energy [0|200]

* Two options for input possible for FacZTra: interpolate or horizon
* If 'horizon' option selected then specify factor for each horizon
* If 'interpolate' option selected then specify factor and depth

table horizon FacZTra    (-)                  Factor for the effect of depth [0|1]
hor pest
1 1
2 1
3 0.5
4 0.3
5 0.3
6 0.3
7 0
8 0
end_table

* Freundlich equilibrium sorption
pH-independent   OptCofFre_pest               pH-dependent, pH-independent, CofFre
1.0              ConLiqRef_pest  (mg.L-1)     Reference conc. in liquid phase [0.1|-]
0.9              ExpFre_pest     (-)          Freundlich sorption exponent [0.1|1.3]

* If pH-independent (use the coefficient for sorption on organic matter):
70.0             KomEql_pest     (L.kg-1)     Coef. eql. sorption on org. matter [0|1e9]
7000.0           KomEqlMax_pest  (L.kg-1)     Coef. eql. sorption on org. matter in dry soil
                                              [0|1e9]

* If pH-dependent (use pKa value and coefficient for sorption on organic matter):
374.7            KomEqlAcid_pest (L.kg-1)     Coef. for eql. sorption on om - acid [0|1e9]
7.46             KomEqlBase_pest (L.kg-1)     Coef. for eql. sorption on om - base [0|1e9]
4.6              pKa_pest        (-)          Coef. for influence of pH on sorption [0|14]
0.0              pHCorrection    (-)          pH correction [-2|1]

* If CofFre (specify the depth dependence and the coefficient for equilibrium sorption):
1.0              KSorEql_pest    (L.kg-1)     Coef. for equilibrium sorption [0|1e9]
0.0              MolEntSor_pest  (kJ.mol-1)
```

```
20.0               TemRefSor_pest  (C)


* Two options for input possible for FacZSor: interpolate or horizon
* If 'horizon' option selected then specify factor for each horizon
* If 'interpolate' option selected then specify factor and depth

table horizon FacZSor       (-)              Factor for the effect of depth [0|1]
hor pest
1 -99
2 -99
3 -99
4 -99
5 -99
6 -99
7 -99
8 -99
end_table


* End If

* Gas/liquid partitioning
0.0               PreVapRef_pest  (Pa)       Saturated vapour pressure [0|2e5]
20.0              TemRefVap_pest  (C)        .. measured at [0|40]
100.0             MolEntVap_pest  (kJ.mol-1) Molar enthalpy of vaporisation [-200|200]
33.0              SlbWatRef_pest  (mg.L-1)   Solubility in water [1e-9|1e6]
20.0              TemRefSlb_pest  (C)        .. measured at [0|40]
40.0              MolEntSlb_pest  (kJ.mol-1) Molar enthalpy of dissolution [-200|200]

* Non-equilibrium sorption
0.00              CofDesRat_pest  (d-1)      Desorption rate coefficient [0|0.5]
0.5               FacSorNeqEql_pest (-)      CofFreNeq/CofFreEql [0|-]

* Uptake
0.5               FacUpt_pest     (-)        Coefficient for uptake by plant [0|10]

* Canopy processes
Lumped            OptDspCrp_pest             Lumped, Specified or Calculated

* If Lumped:
1.d6              DT50DspCrp_pest (d)        Half-life at crop surface [1|1e6]

* If Specified:
1.d6              DT50PenCrp_pest  (d)       Half-life due to penetration [1|1e6]
1.d6              DT50VolCrp_pest  (d)       Half-life due to volatilization [1|1e6]
1.d6              DT50TraCrp_pest  (d)       Half-life due to transformation [1|1e6]

* If Calculated:
1.d6              DT50PenCrp_pest  (d)       Half-life due to penetration [1|1e6]
1.d6              DT50TraCrp_pest  (d)       Half-life due to photo-transformation [1|1e6]
500.0             RadGloRef        (W.m-2)   Global solar radiation for DT50TraCrp
0.0               FraDepRex        (-)       Fraction of deposit with reduced exposure
0.2               FacTraDepRex     (-)       Factor for the effect of restricted exposure
of
                                            deposit on transformation
0.2               FacVolDepRex     (-)       Factor for the effect of restricted exposure
of
                                            deposit on volatilisation
0.2               FacPenDepRex     (-)       Factor for the effect of restricted exposure
of
                                            deposit on penetration
0.2               FacWasDepRex     (-)       Factor for the effect of restricted exposure
of
                                            deposit on wash-off
* End If

1.d-4             FacWasCrp_pest   (m-1)     Wash-off factor [1e-6|0.1]

* Diffusion of solute in liquid and gas phases
4.3d-5            CofDifWatRef_pest (m2.d-1) Reference diff. coeff. in water [10e-5|3e-4]
0.43              CofDifAirRef_pest (m2.d-1) Reference diff. coeff. in air [0.1|3]
20.0              TemRefDif_pest  (C)        Diff. coeff measured at temperature [10|30]

*---------------------------------------------------------------------------------------
* Section 6: Management section
* Description
*---------------------------------------------------------------------------------------

1.0               ZTgt            (m)        Depth of target layer [0.1|Z(N)-1]
1                 DelTimEvt       (a)        Repeat interval of events [NoRepeat|1|2|3]

* Event table:
```

```
* Column 1: Date* Column 2: Event type: AppSolSur, AppSolInj, AppSolTil, AppCrpUsr,
AppCrpLAI
* and ApplfLess
* AppSolSur, AppSolInj, AppSolTil cannot be combined with OptSys set to PlantOnly
* Application to stem : to be added
* If relative date then format is xx-yyy-zzz
*     xx : cropnumber in calendar year
*     yyy: event, Emg (=Emergence) or Har (=Harvest)
* If absolute then format is dd-mmm-yyyy (day – month – year), e.g. 07-Jun-1980
*     zzz: days before event (-zzz) or after event (+zzz)
* If Event = AppSolSur (soil surface application):
* Column 3: Dosage (kg/ha) [0|-]

* If EventType = AppCrp (application to the crop canopy):
* Column 3: Dosage (kg/ha) [0|-]
* Column 4: Optional: Fraction of dosage applied to the crop canopy (-) [0|1]
* Column 5: Optional: Ffield – fraction of dosage lost by fast dissipation (-) [0|1]
*          Required for application by spraying; not required for application by
*          injection (AppSolInj) or incorporation (AppSolTil)

* If EventType = AppLfLess (application to the stem):
* Column 3: Dosage (kg/ha) [0|-]
* Column 4: Fraction of dosage intercepted by stem (-) [0|1]
* Column 5: Ffield – fraction of dosage lost by fast dissipation (-) [0|1]
* Column 5 is only required for ExposureType 'SoilExposure'
* End If

table Applications
01-Emg-001 AppSolSur 1.0
end_table

* Tillage table - can be empty
* Specify date (dd-mmm-yyy) or day in year (dd-mmm) and tillage depth (m)
* table TillageDates
* 15-Oct 0.2
* end_table
* Tillage cannot be combined with OptSys set to PlantOnly

table TillageDates
15-Oct  0.20
end_table


*-------------------------------------------------------------------------------------------
* Section 7: Initial and boundary conditions of pesticide fate model
* Description
*-------------------------------------------------------------------------------------------
* Initial conditions                        Concentration in equilibrium domain [0|-]

* Two options for input possible: interpolate or horizon
* If 'horizon' option selected then specify content for each horizon
* If 'interpolate' option selected then specify content and depth
* If metabolites are included then initial contents for these substances are set to zero.

table interpolate CntSysEql        (mg.kg-1)
0.0000   0.000
3.2000   0.000
end_table

* Initial conditions                        Concentration in non-equil. domain [0|-]
* If using metabolites, ConSysNeq should be specified for all metabolites
table interpolate CntSysNeq        (mg.kg-1)
0.0000   0.000
3.2000   0.000
end_table

* Upper boundary flux                       [0|-]
table    FlmDep   (kg.ha-1.d-1)
01-Jan-1986  0.0
31-Dec-2005  0.0
end_table


*-------------------------------------------------------------------------------------------
* Section 8: Crop section
* Description
*-------------------------------------------------------------------------------------------

Yes              RepeatCrops              Repeat crop table: Yes or No

* Emergence and harvest date of crop.
* Note: Length of growing season must be constant for one crop
```

```
* If repeat crops: Specification of year not required
table  Crops
15-Apr    08-Oct   SUGARBEET1
end_table

* Crop cycle fixed or variable (calculated from temperature sum)
Fixed    OptLenCrp                          Fixed or Variable

* If OptLenCrp = Variable:
0.0            TemSumSta_SUGARBEET1    (C)       Start value of temperature sum [-10|20]
0.0            TemSumEmgAnt_SUGARBEET1  (C)      Sum from emergence to anthesis [0|1e4]
0.0            TemSumAntMat_SUGARBEET1  (C)      Sum from anthesis to maturity  [0|1e4]

* End If

If only plant compartment is considered (OptSys set to 'PlantOnly') then specify fraction of
soil covered by the crop
0.765          FraCovCrpInp (-)      Fraction of soil covered by the crop [0|1]
End if

* Crop parameters as a function of development stage
* Column 1: Development stage: 0 = emergence; 1 = harvest (-)          [0|1]
* Column 2: LAI: Leaf Area Index                          (m2.m-2)     [0|12]
* Column 3: FacCrp: Crop factor                           (-)          [0|2]
* Column 4: ZRoot: Rooting depth                          (m)          [0|10]
* Column 5: HeightCrp:  Crop height                       (m)          [0|10]
*      LAI   FacCrp  ZRoot  HeightCrp

table  CrpPar_SUGARBEET1
0.0    0.0   1.0    0.0    0.0
0.78   4.2   0.87   1.2    0.0
1.0    4.2   0.87   1.2    0.0
end_table

* Root density table (first column is relative depth)
* Column 1: Relative depth 0 = soil surface; 1 = DepRoot  (-)          [0|1]
* Column 2: Root density distribution                     (-)          [0|1]
Table RootDensity_SUGARBEET1
0.00        1.00
1.00        1.00
end_table

* Crop water use
-10.0          HLim1_SUGARBEET1 (cm)      Anaerobiosis point  [-100|0]
-25.0          HLim2_SUGARBEET1 (cm)      Wet reduction point [-1000|0]
-320.0         HLim3U_SUGARBEET1 (cm)     Dry reduction point [-10000|0]
-600.0         HLim3L_SUGARBEET1 (cm)     Dry reduction point [-10000|0]
-16000.0       HLim4_SUGARBEET1 (cm)      Wilting point       [-16000|0]

70.0           RstEvpCrp_SUGARBEET1 (s.m-1)  Min. canopy resistance [0|1000]
0.39           CofExtDif_SUGARBEET1 (-)
1.0            CofExtDir_SUGARBEET1 (-)
0.2            ZTensioMeter_SUGARBEET1 (m)
0.0            FraCovStm_SUGARBEET1 (-)    Soil cover fraction for crop without leaves
-100.0         PreHeaIrrSta_SUGARBEET1 (cm)
1.d-4          CofIntCrp_SUGARBEET1    (cm) Constant in Braden eq for interception [0|1]
15.0           IrgThreshold_SUGARBEET1 (mm) Threshold of moisture deficit to allow
                                            irrigation

*-------------------------------------------------------------------------------------
* Section 9: Output control
* Description
*-------------------------------------------------------------------------------------

* First, specify the time format in the output file:
* DaysFromSta  : Print number of days since start of simulation
* DaysFrom1900 : Print number of days since 1900
* Years        : Print years
DaysFromSta    DateFormat                Format of time column in output file
Yes            OptDelOutFiles
Yes            PrintCumulatives

* Specify type of report required
* Leaching report is not relevant if only Plant compartment is considered

* If ExposureType set to 'Groundwater' then LeachingReport set to Yes, else set to No
* If ExposureType set to 'SoilExposure' then SoilReport set to Yes, else set to No
* If ExposureType set to 'Other', then LeachingReport, SoilReport, DrainageReport and
* AirReport set to No
Yes            LeachingReport            Summary report for leaching assessment
No             DrainageReport            Summary report for drainage assessment
No             AirReport                 Summary report for volatilisation assessment
```

```
No              SoilReport                      Summary report for soil exposure assessment

* If ExposureType set to 'SoilExposure' then specify IntPostApp
* IntPostApp - Interval (days) after last application for additional output on soil exposure
124             IntPostApp (d)                  Interval (days) after last application

* If OptReport set to SoilReport
0.0             ZEADTop         (m)     Depth of the top of the layer for exposure of
                                        soil organisms (Ecological Averaging Depth)
0.2             ZEADBot         (m)     Depth of the bottom of the layer for exposure
of
                                        soil organisms (Ecological Averaging Depth)

* Else
0.2             ThiLayPer       (m)     Target depth for persistence
* End if

If LeachingReport set to 'Yes' then specify target percentile
80.0            TargetPercentile     (%)   Percentile for leaching assessment
End if

* Specify dates for vertical profiles of main state variables, e.g. concentration in liquid
* phase; table can be empty
table VerticalProfiles
end_table

* Format of the ordinary output - use FORTRAN notation:
* e is scientific notation, g = general is general notation
* Then follow the number of positions
* Then the number of digits
g12.4           RealFormat                      Format of ordinary output


* If OptSys is set to 'All' (Soil and Plant) then specify the nodal heights for which output
is requested
* Options are 'table', None or All
table OutputDepths (m)
0.05
0.1
0.2
0.3
0.4
0.5
0.75
1.0
2.0
end_table

* Finally, specify for all variables whether output is wanted (Yes or No)
* As PEARL can potentially generate large output files, it is recommended to minimise
* the number of output variables

* Section I : Output from the SWAP model, version 2.0.9e

* Meteorological data
No              print_VelWnd           wind speed
No              print_TemAir           air temperature

* General variables
No              print_GrwLev           Groundwater level (m)
No              print_LAI              Leaf Area Index (m2.m-2)
No              print_ZRoot            Rooting depth (m)
No              print_FacCrpEvp        Crop factor (-)
No              print_FraCovCrp        Soil cover (-)
No              print_AvoLiqErr        Water balance error (m)
No              print_StoCap           Phreatic storage capacity (m3.m-2)
No              print_AvoLiqSol        Amount of water in soil
No              print_ZPnd             Ponding depth (m)

* If OptMacropore set to 'Yes'
No              print_AvoMacIca
No              print_AvoMacByp
No              print_AvoLiqIca
No              print_AvoLiqByp
No              print_GrwLevByp
* End if

* State variables
No              print_Tem              Soil temperature (C)
No              print_Eps              Volumic air content (m3.m-3)
No              print_Theta            Volumic soil water content (m3.m-3)
No              print_PreHea           Soil water pressure head (m)
```

```
* Volumic volume rates (m3.m-3.d-1)
No              print_VvrLiqDra        Volumic volume rate of drainage
No              print_VvrLiqUpt        Volume flux of water uptake

* If OptMacropore set to 'Yes'
No              print_VvrLiqDraByp
No              print_VvrLiqMicByp
No              print_VvrLiqMicIca
* End if


* Volume fluxes (m3.m-2.d-1)
No              print_FlvLiq           Volume flux of vertical soil water flow
No              print_FlvLiqPrc        Volume flux of precipitation
No              print_FlvLiqIrr        Volume flux of water in irrigation
No              print_FlvLiqLbo        Volume flux of water leaching from the soil system
No              print_FlvLiqInf        Volume flux at lower boundary (m.d-1)
No              print_FlvLiqEvpIntPrc  Evaporation flux of intercepted rainfall
No              print_FlvLiqEvpIntIrr  Evaporation flux of intercepted irrigation
No              print_FlvLiqEvpSol     Volume flux of evaporation from the soil surface
No              print_FlvLiqEvpSolPot  Idem, potential
No              print_FlvLiqTrp        Volume flux of transpiration by plant roots
No              print_FlvLiqTrpPot     Idem, potential
No              print_FlvLiqCanDrp     Volume flux of canopy drip

* If drainage is considered: OptDra >= 1
No              print_FlvLiqDra_1      Volume flux of drainage to level 1
No              print_FlvLiqDra_2      Volume flux of drainage to level 2
No              print_FlvLiqDra_3      Volume flux of drainage to level 3
No              print_FlvLiqDra_4      Volume flux of drainage to level 4
No              print_FlvLiqDra_5      Volume flux of drainage to level 5
No              print_FlvLiqDraTot_1   Volume flux of lateral discharge - level 1 (m.d-1)
                                       Drainage from micropore and macropore domain
No              print_FlvLiqDraTot_2   Volume flux of lateral discharge - level 2 (m.d-1)
                                       Drainage from micropore and macropore domain
No              print_FlvLiqDraTot_3   Volume flux of lateral discharge - level 3 (m.d-1)
                                       Drainage from micropore and macropore domain
* End if

No              print_FlvLiqGrw        Volume flux groundwater recharge
No              print_FlvLiqGrwSur     Groundwater flux (m.d-1)

* If OptMacropore set to 'Yes'
No              print_FlvLiqInfPrcIca    Direct infiltration into ic domain (m.d-1)
No              print_FlvLiqInfRunOffIca Infiltration by runoff into ic domain (m.d-1)
No              print_FlvLiqInfPrcByp    Direct infiltration into bypass domain (m.d-1)
No              print_FlvLiqInfRunOffByp Infiltration by runoff into bypass domain (m.d-1)
No              print_FlvLiqDraByp       Volume flux of drainage from bypass domain (m.d-
1)
No              print_FlvLiqMicByp       Exchange flux between micropores and bypass (m.d-
1)
No              print_FlvLiqBypMic       Exchange flux between bypass and matrix (m.d-1)
No              print_FlvLiqMicIca       Exchange flux between micropores and ic dom.(m.d-
1)
No              print_FlvLiqIcaMic       Exchange flux between ica and matrix  (m.d-1)
* End if


* Section II : Output from the PEARL model
* Remark: All fluxes are averages over the print interval
*--------------------------------------------------------
* Time step
No              print_DelTimPrl        Average time-step during the print interval (d)

* Section II a: Output for the soil compartment; OptSys = All (Plant and Soil compartment)

No              print_AmaErrMic        Areic numerical mass error in soil matrix
                                        (micropore domain


* Mass balance (kg.m-2)
No              print_AmaEqlPro        Areic mass in equilibrium domain of profile
No              print_AmaEqlTil        Areic mass in equilibrium domain of tillage layer
No              print_AmaEqlTgt        Areic mass in equilibrium domain of target layer
No              print_AmaNeqPro        Areic mass in non-eql. domain of profile
No              print_AmaNeqTil        Areic mass in non-eql. domain of tillage layer
No              print_AmaNeqTgt        Areic mass in non-eql. domain of target layer
No              print_AmaSysPro        Areic mass of pesticide in the system
No              print_AmaSysTil        Areic mass of pesticide in the tillage layer
No              print_AmaSysTgt        Areic mass of pesticide in the target layer
No              print_AmaAppSol        Areic mass applied to the soil system
No              print_AmaForPro        Areic mass of formation
```

```
No                print_AmaTraPro      Areic mass of pesticide transformation
No                print_AmaUptPro      Areic mass of pesticide uptake
No                print_AmaRunOff      Areic mass of runoff from the field
No                print_AmaSolSur      Areic mass of deposit at soil surface

* If OptMacropore set to 'Yes'
No                print_AmaInfRunOffByp  Areic mass of runoff infiltrating the bypass domain
No                print_AmaInfRunOffIca  Areic mass of runoff infiltrating the ic domain
No                print_AmaDraByp      Areic mass of drainage from the bypass domain
No                print_AmaDraPro      Areic mass of drainage from the micropore domain
No                print_AmaMicIca      Areic mass of exchange between ica and matrix
No                print_AmaMicByp      Areic mass of exchange between bypass and matrix
No                print_AmaIcaMic      Areic mass of exchange between ica and matrix
No                print_AmaBypMic      Areic mass of exchange between bypass and matrix
No                print_AmaByp         Areic mass in the bypass domain
No                print_AmaIca         Areic mass in the internal catchment domain
* End if


* If drainage is considered: OptDra >= 1
No                print_AmaDra_1       Areic mass of drainage to level 1
No                print_AmaDra_2       Areic mass of drainage to level 2
No                print_AmaDra_3       Areic mass of drainage to level 3
No                print_AmaDra_4       Areic mass of drainage to level 4
No                print_AmaDra_5       Areic mass of drainage to level 5
No                print_AmaDraPro      Areic mass of lateral discharge
* End if


* Pesticide concentrations (kg.m-3) and contents (kg.kg-1)
No                print_ConLiq         Concentration in liquid phase
No                print_ConGas         Concentration in gas phase
No                print_ConSysEql      Concentration in equilibrium domain
No                print_ConSysNeq      Concentration in non-equilibrium domain
No                print_ConSys         Concentration in the soil system
No                print_ConLiqSatAvg   Avg. conc.in liq. phase between 1-2 m
No                print_ConLiqLbo      Concentration in percolate

* If drainage is considered: OptDra >= 1
No                print_ConLiqDra      Concentration in drainage water
No                print_ConLiqDra_1    Concentration in drainage water, system 1
No                print_ConLiqDra_2    Concentration in drainage water, system 2
No                print_ConLiqDra_3    Concentration in drainage water, system 3
No                print_ConLiqDra_4    Concentration in drainage water, system 4
No                print_ConLiqDra_5    Concentration in drainage water, system 5
* End if


* If OptAux = 2 or OptAux = 3 then
No                print_ConLiqDitch_1  Concentration in surface water from level 1
No                print_ConLiqDitch_2  Concentration in surface water from level 2
No                print_ConLiqDitch_3  Concentration in surface water from level 3
* End if

* If OptMacropore set to 'Yes'
No                print_ConLiqByp      Concentration in the bypass domain
No                print_ConLiqIca      Concentration in the internal catchment domain
No                print_ConLiqTot      Total concentration (mean of matrix and macropore)
No                print_ConLiqDraByp   Concentration in drainage water from bypass domain
* End if

* If paddy water layer is considered: OptPaddy set to 'Yes'
No                print_ConLiqWatLay      Concentration in the paddy water layer
No                print_ConLiqWatLayCur   Current concentration in the paddy water layer
No                print_ConLiqRunWatLay   Concentration in run-off water
* End if


* If OptReport set to SoilReport
No                print_ConLiqEAD      Liquid concentration in target layer soil exposure
No                print_CntSysEAD      Content in layer soil exposure
No                print_ConLiqTWA7D()  Time-weighted liquid concentration for 7 day
                                       period in persistency layer
No                print_ConLiqTWA14D() Time-weighted liquid concentration for 14 day
                                       period in persistency layer


No                print_ConLiqTWA21D() Time-weighted liquid concentration for 21 day
                                       period in persistency layer
No                print_ConLiqTWA28D() Time-weighted liquid concentration for 28 day
                                       period in persistency layer
No                print_ConLiqTWA56D() Time-weighted liquid concentration for 56 day
```

```
                                                 period in persistency layer
No                print_ConLiqTWA100D()   Time-weighted liquid concentration for 100 day
                                                 period in persistency layer
No                print_CntSysTWA7D()     Time-weighted total content for 7 day period in
                                                 persistency layer
No                print_CntSysTWA14D()    Time-weighted total content for 14 day period in
                                                 persistency layer
No                print_CntSysTWA21D()    Time-weighted total content for 21 day period in
                                                 persistency layer
No                print_CntSysTWA28D()    Time-weighted total content for 28 day period in
                                                 persistency layer
No                print_CntSysTWA56D()    Time-weighted total content for 56 day period in
                                                 persistency layer
No                print_CntSysTWA100D()   Time-weighted total content for 56 day period in
                                                 persistency layer
* Else

No                print_ConLiqPer         Liquid concentration in persistency layer
No                print_CntSysPer         Total content in persistency layer
* End if

* Pesticide mass fluxes (kg.m-2.d-1)
No                print_FlmLiq            Pesticide mass flux in liquid phase
No                print_FlmGas            Pesticide mass flux in gas phase
No                print_FlmSys            Total pesticide mass flux (FlmLig+FlmGas)
No                print_FlmLiqLbo         Accumulated mass flux at the lower boundary
No                print_FlmLiqInfSys      Accumulated mass flux of pesticide infiltration
No                print_FlmGasVol         Accumulated mass flux of pesticide volatilisation

* Volatilisation concepts
* if OptTraRes = 1, concept of laminar air boundary resistance
No                print_RstAirLam         Resistance to transport through laminar air layer
                                                 (s.m-1)
* End if

* If OptTraRes = 2, concept of aerodynamic resistance
No                print_RstAer            aerodynamic resistance
No                print_RstBou            boundary resistance
No                print_VelFriLcl         friction velocity
* End if


* End of Section II a

* Section II b: Output for the plant compartment
* Remark: OptSys can be 'All' or 'PlantOnly'
*---------------------------------------------------------

* General
*-------------------
No                print_AmaCrp            Areic mass of pesticide at the canopy
No                print_AmaAppCrp         Areic mass of pesticide applied to the canopy
No                print_AmaDspCrp         Areic mass rate of pesticide dissipation
No                print_AmaHarCrp         Areic mass rate of pesticide removal by harvest
No                print_AmaWasCrp         Areic mass rate of pesticide wash-off
No                print_FlmDepCrp         Areic mass rate of pesticide deposited on canopy

* Specific
*-------------------

If competing processes are considered: OptDspCrp > 1
No                print_AmaVolCrp         Areic mass of pesticide volatilised from crop
canopy
No                print_AmaPenCrp         Areic mass penetrated into the crop canopy
No                print_AmaTraCrp         Areic mass transformed on the crop canopy
End if

If competing processes are considered and volatilisation dependent on meteorological
conditions: OptDspCrp = 3
No                print_AmaCrpFex         Areic mass fully exposed at the crop canopy
No                print_AmaCrpRex         Areic mass with reduced exposure at the crop canopy
No                print_AmaVolCrpFex      Areic mass of pesticide volatilised
No                print_AmaVolCrpRex      Areic mass of pesticide volatilised from deposit
with
                                                 reduced exposure
No                print_AmaWasCrpFex      Areic mass of wash-off from fully exposed deposit
No                print_AmaWasCrpRex      Areic mass of wash-off from deposit with reduced
                                                 exposure

No                print_AmaPenCrpFex      Areic mass of fully exposed pesticide penetrated
into
                                                 the plant
No                print_AmaPenCrpRex      Areic mass of pesticide penetrated into the plant
```

```
                                    from deposit with reduced exposure
No                 print_AmaTraCrpFex    Areic mass of fully exposed pesticide transformed
on
                                    the plant surface
No                 print_AmaTraCrpRex    Areic mass of restrictedly exposed pesticide
                                    transformed on the plant surface
End if
* End of Section II b

*-------------------------------------------------------------------------------
* End of PEARL input file
*-------------------------------------------------------------------------------
```

Annex 2   Description of the weather data file

The weather data file consists of 11 columns. Depending on the value of OptEvp (see page 24), one or more columns can be left blank. See Table A 2.1

Table A 2.1 *Contents of the weather data file*

Column name	Required in the case of OptEvp =		
	Penman	Makkink	Input
Meteostation code. The Meteostation code must be the same as the code specified in the Meteostation record of the PEARL file	Yes	Yes	Yes
Day, between 1 and 31	Yes	Yes	Yes
Month, between 1 and 12	Yes	Yes	Yes
Year, between 1900 and 3000	Yes	Yes	Yes
Daily global radiation (kJ m^{-2} d^{-1}), between 0 and 5 10^6	Yes	Yes	No
Minimum daily temperature (^{o}C), between -50 and 35	Yes	Yes	Yes
Maximum daily temperature (^{o}C), between -30 and 60	Yes	Yes	Yes
Average vapor pressure (kPa), between 0 and 10	Yes	No	No
Average windspeed (m s^{-1}), between 0 and 50	Yes	No	No
Daily precipitation (mm d^{-1}), between 0 and 1000	Yes	Yes	Yes
Reference evapotranspiration (mm d^{-1}), between 0 and 100	No	No	Yes

If a column is left blank, -99.9 should be specified.

Annex 3　The format of the PERSAM transfer (ptf) file

```
*-----------------------------------------------------------------
* PERSAM Transfer file
* Generated on 09/10/2019_11:02
*-----------------------------------------------------------------
South RegZone Regulatory zone (options: North, Centre, South)
TotSol TypeOfEP Type of endpoint (options: TotSol, PoreWat)
5392000_2285000 Location X/Y coordinates
P SubstanceAss Substance assessed (options: P, M1A, M1B, M1C, M1D, M2A, M2B, M2C,
M2D)
1 fRef (-) Refinement factor for final PEC
10 PERSAMCropNr PERSAM crop number
VeryFine SoilTypeID Soil texture (options: Coarse, Medium, MediumFine, Fine,
VeryFine, Organic)
0.0325 CntOmSca (kg.kg-1) Topsoil organic matter content
6.90 pHInp (-) Topsoil pH
594 Prc (mm) Mean annual precipitation
10.1 Temp (C) Mean annual temperature
substance_4 Name_P Substance name
-99 Name_M1A ------II------
-99 Name_M1B ------II------
-99 Name_M1C ------II------
-99 Name_M1D ------II------
-99 Name_M2A ------II------
-99 Name_M2B ------II------
-99 Name_M2C ------II------
-99 Name_M2D ------II------
300 MolMas_P (g.mol-1) Molar mass
-99 MolMas_M1A (g.mol-1) ----II----
-99 MolMas_M1B (g.mol-1) ----II----
-99 MolMas_M1C (g.mol-1) ----II----
-99 MolMas_M1D (g.mol-1) ----II----
-99 MolMas_M2A (g.mol-1) ----II----
-99 MolMas_M2B (g.mol-1) ----II----
-99 MolMas_M2C (g.mol-1) ----II----
-99 MolMas_M2D (g.mol-1) ----II----
-99 P -> M1A (-) Molar formation fraction
-99 P -> M1B (-) -----------II-----------
-99 P -> M1C (-) -----------II-----------
-99 P -> M1D (-) -----------II-----------
-99 M1A -> M2A (-) -----------II-----------
-99 M1A -> M2B (-) -----------II-----------
-99 M1A -> M2C (-) -----------II-----------
-99 M1A -> M2D (-) -----------II-----------
-99 M1B -> M2A (-) -----------II-----------
-99 M1B -> M2B (-) -----------II-----------
-99 M1B -> M2C (-) -----------II-----------
-99 M1B -> M2D (-) -----------II-----------
-99 M1C -> M2A (-) -----------II-----------
-99 M1C -> M2B (-) -----------II-----------
-99 M1C -> M2C (-) -----------II-----------
-99 M1C -> M2D (-) -----------II-----------
-99 M1D -> M2A (-) -----------II-----------
-99 M1D -> M2B (-) -----------II-----------
-99 M1D -> M2C (-) -----------II-----------
-99 M1D -> M2D (-) -----------II-----------
31 DT50Ref_P (d) Half-life time
-99 DT50Ref_M1A (d) ------II------
-99 DT50Ref_M1B (d) ------II------
-99 DT50Ref_M1C (d) ------II------
-99 DT50Ref_M1D (d) ------II------
-99 DT50Ref_M2A (d) ------II------
-99 DT50Ref_M2B (d) ------II------
-99 DT50Ref_M2C (d) ------II------
-99 DT50Ref_M2D (d) ------II------
65.4 MolEntTra_P (kJ.mol-1) Molar activation energy
```

```
-99 MolEntTra_M1A (kJ.mol-1) ----------II-----------
-99 MolEntTra_M1B (kJ.mol-1) ----------II-----------
-99 MolEntTra_M1C (kJ.mol-1) ----------II-----------
-99 MolEntTra_M1D (kJ.mol-1) ----------II-----------
-99 MolEntTra_M2A (kJ.mol-1) ----------II-----------
-99 MolEntTra_M2B (kJ.mol-1) ----------II-----------
-99 MolEntTra_M2C (kJ.mol-1) ----------II-----------
-99 MolEntTra_M2D (kJ.mol-1) ----------II-----------
31 KomEql_P (L.kg-1) Coef. eql. sorption on org. matter
-99 KomEql_M1A (L.kg-1) ----------------II----------------
-99 KomEql_M1B (L.kg-1) ----------------II----------------
-99 KomEql_M1C (L.kg-1) ----------------II----------------
-99 KomEql_M1D (L.kg-1) ----------------II----------------
-99 KomEql_M2A (L.kg-1) ----------------II----------------
-99 KomEql_M2B (L.kg-1) ----------------II----------------
-99 KomEql_M2C (L.kg-1) ---------------II---------------
-99 KomEql_M2D (L.kg-1) ---------------II---------------
0.00E0 ZEADTop (m) Top of the evaluation depth
0.0500 ZEADBot (m) Bottom of the evaluation depth
1 DelTimEvt (a) Repeat interval of events (options: 1, 2, 3)
49 IntPostApp (d) Time interval for post-application PEC (days after last
application)
AppCrpUsr OptApp Application (options: AppSolSur, AppCrpUsr, AppSolInj,
AppSolTil)
0 ZApp (m) Application depth (incorporation or injection)
3 NrApp (-) Number of applications events
* Application table (day - rate (kg.ha-1) - crop interception (fraction of
dosage, dimensionless))

table Applications
0 1.200000000000000 0.300
14 0.8000000000000000 0.600
21 0.4000000000000000 0.600
end_table
```

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