



Manual GEM 1.1.1

Greenhouse Emission Model, exposure assessment tool for Plant Protection Products used in greenhouse crops

E.L. Wipfler, C. Vink, M.M.S. ter Horst & A. de Jong



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Software manual of the software instrument 'Greenhouse Emission Model' (GEM1.1.1). GEM calculates exposure concentrations of Plant Protection Products (PPP) in surface water and leaching to groundwater as part of the environmental risk assessment. The PPP is applied in greenhouses on soil bound and soilless cultivated crops.

Software handleiding van het software instrument 'Greenhouse Emission Model' (GEM1.1.1). GEM berekent blootstellingsconcentraties van gewasbeschermingsmiddelen in oppervlaktewater en emissie naar grondwater als onderdeel van de milieurisicobeoordeling. De gewasbeschermingsmiddelen worden toegepast in grondgebonden teelten en substraatteelten.

Keywords: pesticides, pesticide fate models, greenhouse emissions, pesticide environmental risk assessment

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Preface

In 2010, the Dutch ministries of Economic Affairs and Infrastructure & the Environment charged two working groups to develop new exposure scenarios for the environmental risk assessment of Plant Protection Products (PPP) used in greenhouse horticulture. The task of the first working group was to develop scenarios for PPP use in soilless cultivation and of the second to develop scenarios for PPP use in soil-bound cultivation. These two working groups developed their views and approaches towards the development of these scenarios, which reflect the current practices as well as the state-of-the-art scientific knowledge regarding the development of scenarios and the emission of chemicals towards groundwater and surface water.

This manual provides a guide for the user of the Greenhouse Emission Model (GEM) instrument. The exposure assessment instrument incorporates the new greenhouse horticulture scenarios as developed by the two working groups. It is intended to be used in the Dutch registration process. As far as we know, this is the first instrument that is specifically dedicated to greenhouse horticulture to be used in the environmental risk assessment as part of the PPP registration process. In the coming years the developments in this important Dutch economic sector will continue. It is expected that this instrument will develop further following the developments and new scientific insights.

Samenvatting

Deze handleiding is ter ondersteuning van de gebruiker van het software instrument GEM 1.1.1 (Greenhouse Emission Model 1.1.1). GEM 1.1.1 bevat de Nederlandse glastuinbouw blootstellingsscenario's zoals beschreven in Van der Linden *et al.* (2015) en Wipfler *et al.* (2015a) en berekent blootstellingconcentraties van gewasbeschermingsmiddelen voor de beschermdoelen: 'Aquatisch ecosysteem' en 'Grondwater als bron van drinkwater' als onderdeel van de milieurisicobeoordeling. Het instrument is ontwikkeld om te worden gebruikt bij de toelating van gewasbeschermingsmiddelen in Nederland. Wij raden aan om voorafgaand aan de toepassing van het instrument de bijbehorende scenario rapporten goed door te lezen.

GEM 1.1.1 is hiërarchisch georganiseerd in projecten (*projects*) en beoordelingen (*assessments*). Een project bevat een aantal beoordelingen met dezelfde teelt-beoordelingcombinatie. De gebruiker kan kiezen welke combinatie moet worden beschouwd:

- Oppervlaktewaterbeoordeling voor gewasbeschermingsmiddelen toegepast in substraat teelt
- Oppervlaktewaterbeoordeling voor gewasbeschermingsmiddelen toegepast in grondgebonden teelt
- Grondwaterbeoordeling voor gewasbeschermingsmiddelen toegepast in grondgebonden teelt

Een beoordeling bestaat uit een vast scenario deel en een door de gebruiker in te voeren deel. De gebruiker kan zelf stoffen en stoffeigenschappen invoeren, gewassen selecteren en toedieningsschema's invoeren. De (vaste) scenario eigenschappen zijn voor elk van de teelt-beoordelingcombinaties verschillend. Ook de modellen die achtereenvolgens worden aangeroepen om de blootstellingconcentratie te berekenen verschillen per teelt-beoordelingcombinatie. Deze zijn het WATERSTROMEN model, het Substance Emission Model, PEARL en TOXSWA.

GEM heeft twee hoofdschermen: het projectenscherm en het beoordelings scherm. Het projectenscherm geeft de mogelijkheid om projecten te organiseren en het beoordelings scherm geeft de mogelijkheid om het gewas, de stof en het applicatieschema te kiezen. Ook kunnen eventuele mitigatieopties worden ingevoerd (alleen voor substraatteelt) en uitvoeropties worden geselecteerd. Daarnaast kan via het beoordelings scherm de berekening van de blootstellingsconcentraties worden gestart en de resultaten worden bekeken in de vorm van een beoordelingsrapportage en figuren.

Voor substraatteelt moet voorafgaand aan de berekeningen het percentiel van de te berekenen concentraties worden geselecteerd. Dit kan ofwel het 50^{ste} ofwel het 90^{ste} percentiel zijn. Voor grondgebondenteelten is het percentiel altijd het 90^{ste} percentiel, zowel voor grondwater als voor oppervlakte water.

Stoffen en stoffeigenschappen worden gemanaged m.b.v. de Substance PlugIN (SPIN) tool. Dit instrument is speciaal ontwikkeld voor het bewaren, invoeren en toegankelijk maken van stoffeigenschappen. SPIN kan ook als *stand-alone* applicatie worden gebruikt en is toegankelijk voor meerdere blootstellingsmodellen zoals SWASH en FOCUS-TOXSWA.

Summary

This manual describes the exposure assessment instrument GEM 1.1.1 (Greenhouse Emission Model 1.1.1) to be used in the Plant Protection Product (PPP) registration process. The tool includes the greenhouse horticulture scenarios for the Netherlands as reported in Van der Linden *et al.* (in prep) and Wipfler *et al.* (2015a). The instrument enables the calculation of the Predicted Environmental Concentration for the protection goals: 'Aquatic ecosystem' and 'Groundwater as source for drinking water'.

The instrument is intended to be used in the Dutch plant protection product registration process. It is recommended to read the corresponding scenario documents before using the GEM instrument.

GEM 1.1.1 organises calculations in *projects* and *assessments*. A project comprises of a series of assessments of the same cultivation-assessment type combination. The user has to choose which cultivation – assessment type combination the project will contain:

- Surface water exposure assessment for PPP used in soilless cultivation
- Surface water exposure assessment for PPP used in soil-bound cultivation
- Leaching assessment to groundwater for PPP used in soil-bound cultivation

Each assessment is composed of *fixed* scenario properties, and *user-defined* substance, crop and application scheme information. Scenario properties differ per cultivation-assessment type combination and for each cultivation – assessment type combination a different series of process models is called to calculate the corresponding Predicted Environmental Concentration. Incorporated models are the WATERSTROMEN model, the Substance Emission Model, PEARL and TOXSWA.

The instrument consists of a Projects form and an Assessment form to manage the projects and assessments. The Projects form enables the user to manage the projects. On the assessment form the user may select a crop and a substance and may define the application management of the PPP. In addition optional mitigation measures may be included (only for soilless cultivation) and output options may be defined. The assessment form facilitates the calculation of the Predicted Environmental Concentrations and the viewing of a summary report and illustrating graphs.

For soilless cultivation either 50th percentile or 90th percentile concentration must be selected as target endpoint of the simulation before starting the calculations. For soil-bound cultivation the Predicted Environmental Concentration is the 90th percentile for both surface water and groundwater.

To manage and edit substance properties, GEM 1.1.1 is connected to the Substance PlugIN (SPIN) tool. This software instrument has been developed to store and manage substance properties. SPIN can be used as a stand-alone application and can be accessed by other pesticide fate models (referred to as host applications) from Alterra Wageningen UR (e.g. SWASH 5.3, FOCUS-TOXSWA 4.4.2).

1 Introduction

1.1 Background

Greenhouse horticulture is an important economic sector for the Netherlands. E.g. greenhouse horticulture accounted for 39 percent of Dutch agricultural production in 2011. The share of horticulture in the total Dutch exports in 2010 was 4%, as part of a total share of agricultural exports of 34% (source: www.hollandtrade.com).

Cropping systems are optimally organized in greenhouses, production is intensive and largely independent of seasonal influences aiming at continuous production. Plant Protection Product (PPP) management is optimized for use in these systems, often leading to frequent application of PPP at high rates.

The environmental risk assessment methodology of Plant Protection Products used in greenhouses has not been changed over the last 30 years. The methodology does not reflect current agricultural practices as it does not account for potential major emission routes to surface water. Neither does it account for the high amounts of irrigation water that increase the potential risk of PPP leaching to groundwater and surface water. Facing high concentrations of PPP in surface waters near greenhouses, the Dutch government considered this situation no longer defensible and therefore charged two working groups to develop exposure assessment scenarios for greenhouse horticulture systems. One working group developed surface water exposure scenarios for soilless crops and one working group developed a groundwater leaching scenario and a surface water exposure scenario, both for soil-bound crops. Scenario development is described in Van der Linden *et al.* (2015) for soilless cultivation and Wipfler *et al.* (2015a) for soil-bound cultivation.

This manual describes the exposure assessment instrument GEM 1.1.1 (Greenhouse Emission Model 1.1.1). The instrument enables the calculation of the Predicted Environmental Concentration for the protection goals: 'Aquatic ecosystem' and 'Groundwater as source for drinking water', while using the scenarios as described in Van der Linden *et al.* (2015) and Wipfler *et al.* (2015a). We strongly recommend to read these documents before using the GEM software.

The instrument is intended to be used in the Dutch PPP authorisation process. The position of the scenarios in a tiered approach has not been decided yet.

Three main types of assessments are incorporated in the GEM instrument:

- Surface water exposure assessment for PPP used in soilless cultivation
- Surface water exposure assessment for PPP used in soil-bound cultivation
- Leaching assessment to groundwater for PPP used in soil-bound cultivation

These will be discussed in the next Sections.

1.2 Surface water exposure scenarios for soilless cultivation

Crops grown on substrate were divided over four categories based on their water requirement and sodium tolerance and dominant growing system. Each of these categories has a specific discharge pattern to the nearby ditch. For each of these categories an exposure scenario was developed by Van der Linden *et al.* (2015). The endpoint of the exposure assessment, i.e. the Predicted Environmental Concentration (PEC), was defined as the target overall percentile annual peak concentration in an

evaluation ditch with a length of 100 m. The target percentile can be either a 50th or a 90th percentile, both options are possible in GEM.

To calculate the surface water concentrations three models must be run in consecutive order as depicted below. The WATERSTROMEN model calculates the water fluxes in the soilless greenhouse system as well as the discharged volumes. The Substance Emission Model calculates the PPP fate in the system and the discharged PPP mass. TOXSWA calculates the PPP concentrations in the receiving ditch while accounting for PPP fate processes such as dilution, degradation and sorption. The models are run over the time period 2000 to 2007 (in total seven years). The PEC is calculated as the target percentile of the seven annual peak surface water concentrations.

In Annex 1 the crops of the "Definitielijst Toepassingsgebieden Gewasbeschermingsmiddelen" (Definition list of areas of application for plant protection products; in this report referred to as the DTG-list) that are grown in substrate are listed. The reference crops that represent the corresponding category is indicated for each of these crops. PPP can be applied to these crops with the nutrient solution, by spraying, fogging or with a low volume mister. To allow for a chronic risk assessment, the Time Weighted Average concentrations calculated for the year that is nearest to the target percentile may be calculated as a secondary endpoint.

Optionally, the effect of the use of an end-of-pipe water treatment facility can be simulated as well, as a mitigation measure for PPP emission to surface water.



1.3 Surface water exposure scenario for soil-bound cultivation

One exposure assessment scenario was derived for all soil-grown crops, based on the model crop: chrysanthemum. The endpoint of the assessments was defined as the 90th overall percentile annual peak concentration in an evaluation ditch with a length of 100 m. The 90th temporal percentile concentration corresponds to the 90th overall percentile concentration.

Three models must be run in consecutive order to calculate the surface water concentration. The SWAP model calculates the hydrology in the greenhouse soil, PEARL calculates the PPP fate in the greenhouse soil and emission to the drains and TOXSWA calculates the PPP concentration in the receiving ditch. The TOXSWA model is run over the time period 2000 to 2007 (in total seven years). The PEC is calculated as the 90th percentile of the seven annual peak surface water concentrations. The PEARL model is run for the period 1981 to 2007. The first six years are indicated as 'warming up period', however output is provided for the entire period. TOXSWA only uses PEARL output of the last seven years as input.

In Annex 1 the crops of the DTG list that are grown in soil are listed. PPP can be applied either to the crop canopy, the soil surface, by incorporation or injection. The assessment is not sensitive to the selected crop; i.e. the scenario is considered representative for all soil-bound crops. To allow for a chronic risk assessment, the Time Weighted Average concentrations calculated for the year that is nearest to the target percentile is calculated as well.



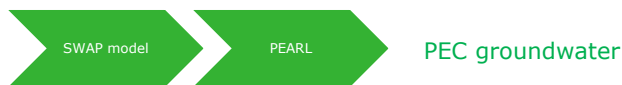
1.4 Groundwater leaching scenario for soil-bound cultivation

One groundwater leaching assessment scenario was derived for all soil-grown crops, based on the model crop: chrysanthemum.

The endpoint of the assessments was defined as the 90th percentile annual average groundwater concentration at 1 m depth. The 90th temporal percentile concentration corresponds to the 90th overall percentile concentration.

Two models need to be run in consecutive order to calculate the groundwater leaching concentration. The SWAP model calculates the hydrology in the greenhouse soil, PEARL simulates the PPP fate in the greenhouse soil and calculates the groundwater concentrations as well as the end point concentration. The models are run over the period 1981 to 2007, with a warming up period of six years.

In Annex 1 the crops of the DTG list that are grown in soil are listed. PPP can be applied either to the crop canopy, the soil surface, by incorporation or injection. The assessment is not sensitive to the selected crop; i.e. the scenario is considered representative for all soil-bound crops.



1.5 Report structure

This report provides a user's guide to the exposure assessment instrument GEM 1.1.1 for soilless as well as soil-bound cultivation in Dutch greenhouses. In Chapter 2 the software and directory structure of GEM is described. The models used to simulate the PPP fate processes and the surface water concentrations are shortly discussed in Chapter 3. Chapter 4 is dedicated to the installation of GEM and starting up issues. The main forms of GEM are discussed in Chapter 5 and 6. In Chapter 7 additional guidance is given to the user.

2 GEM structure

2.1 Software structure

The GEM instrument covers three main types of assessment-cultivation type combinations:

- Surface water exposure assessment for PPP used in soilless cultivation
- Surface water exposure assessment for PPP used in soil-bound cultivation
- Leaching assessment to groundwater for PPP used in soil-bound cultivation

To calculate the Predicted Environmental Concentrations (PECs), a number of hydrological and fate models are run in consecutive order. The models and the sequence of the models differ per assessment-cultivation type. The software shell of GEM takes care that the correct models are run in correct order.

The GEM software structure is shown in Figure 2.1. The Graphical User Interface (GUI) is centrally situated in the figure. The GEM GUI enables the user to select a substance and enter the application and crop information and choose between output options. Scenario-specific properties are fixed and cannot be modified via the GUI. The GEM GUI connects to the GUI of the substance property database SPIN (Substance Plug In, Van Kraalingen *et al.*, 2013) and reads the relevant properties of the selected substance.

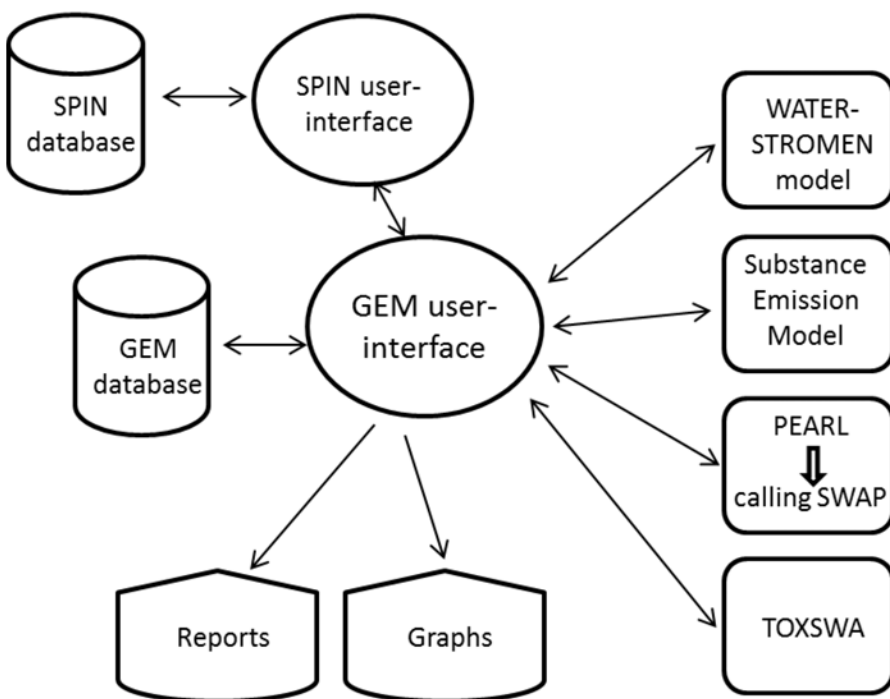


Figure 2.1 Schematic representation of the GEM structure.

The substance properties together with crop and application data are translated into input files for the consecutive models, which are either the WATERSTROMEN model, the Substance Emission Model, PEARL or TOXSWA. GEM communicates with the models by modifying the ASCII input and reading the output files. Some of the output files are optionally used as input files by the next model in line. Once a simulation run is finished, an assessment report, tabulated data and figures of emissions and concentrations can be viewed within the GUI.

SPIN may additionally be started to enter or modify substances. SPIN enables the storage and management of PPP properties in a common database that can be accessed by different host applications from Alterra Wageningen UR. SPIN can also be used as a stand-alone application. Substance properties can be entered and saved on the different tabs in the Edit Substances section of SPIN. For each property an entry field is provided. In case SPIN is accessed via a host application, fields of those properties can be edited only if relevant for the host application; the irrelevant properties are visible but cannot be edited. If SPIN is accessed via GEM, SPIN allows for differentiating between the three cultivation-assessment type combinations, which each have different substance property requirements. SPIN is backwards compatible, which implies that new versions of SPIN can always be used with earlier released host-applications. For further information on SPIN, we refer to Kraalingen *et al.* (2013).

2.2 Hierarchical data structure

The hierarchical data structure of GEM is depicted in Fig. 2.2. GEM model data are organized in *projects* and *assessments*. One project comprises of a series of assessments of the same cultivation-assessment type combination. An assessment is composed of *fixed* scenario properties, and *user defined* information. User defined information is related to substance properties, crop type, application scheme and impact of mitigation measures. The scenario properties differ per cultivation-assessment type combination. The user can select only those crops from the DTG list that are relevant for the cultivation type (i.e. soilless or soilbound) selected (Annex 1). One assessment contains one crop and one substance, but may contain multiple applications with different application types.

Each GEM project or assessment has a unique ID number. ID numbers of GEM projects and assessments are assigned in sequential order of creating the projects or assessments. When defining a new project, previously used project and assessment ID's will not be re-used in the new project (regardless of whether output for that project or assessment exists or whether previously created projects and/or assessments were deleted).

GEM allows the user to select multiple assessments per project for execution, which are calculated in consecutive order.

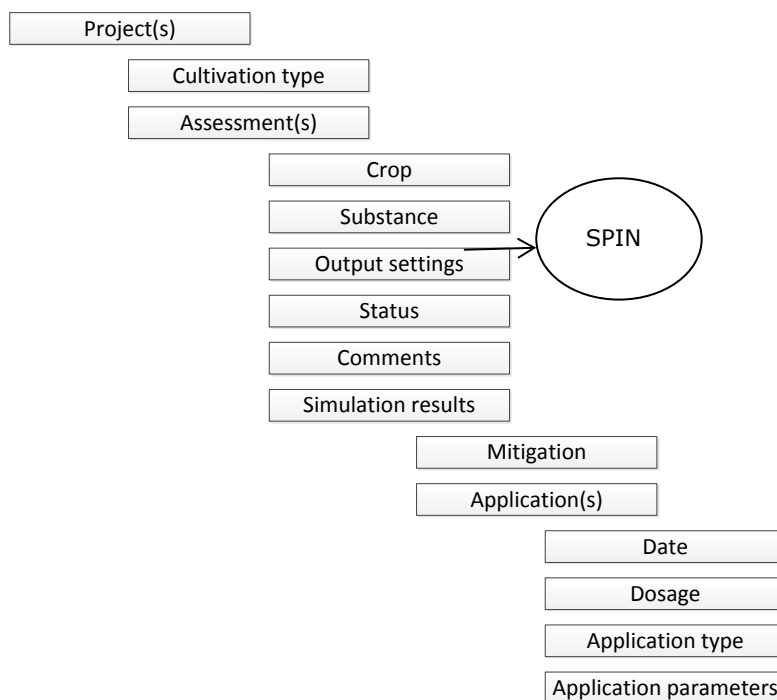


Figure 2.2 Hierarchical data structure of a project. A project has only one cultivation –assessment type combination. It may contain more than one assessment. An assessment contains only one crop and one substance and can contain several applications.

2.3 Directory structure

Communication between GEM and the process models is done by ASCII input and output files. These input and output files are stored in folders. Files that belong to GEM projects are stored in the Projects folder, of which the location must be entered by the user during installation of GEM. ID numbers of GEM projects and assessments correspond to names of subfolders of the Projects folder. The name of the folder is constructed according to the project ID, assessment ID and name of the model. An example of such a folder structure is given in Figure 2.3.

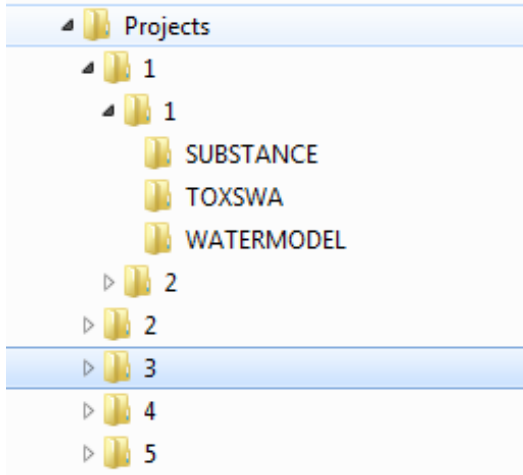


Figure 2.3 Example of the project-assessment Projects folder structure of GEM. Folders 1 to 5 are project folders; assessment folders are subfolders of the project folders. Model simulation results are stored in the subfolders, after the model run is completed.

3 Model descriptions

3.1 WATERSTROMEN

The WATERSTROMEN model (Voogt *et al.*, 2012) calculates fluxes and residence times of water in a greenhouse using substrate as growth medium (soilless cultivation) as well as temperatures. A general description of the water flows in soilless cultivation is given in Figure 3.1. The boundaries of the system are the greenhouse sides, vents and the groundcover. The model accounts also for the area with the fertigation and water treatment equipment. Irrigation and (evapo-) transpiration are the main water flow drivers. Irrigation water is considered as input to the system and may originate from various sources, each of them having its own dynamics and constraints. Precipitation on the greenhouse roof is stored in a reservoir and used for crop irrigation. Other sources considered are e.g. tap water or groundwater. The water balance's main sinks are (i) the crop water uptake, i.e. for growth and for transpiration and (ii) waste-water flows: the filter cleaning, leakages and discharge of recirculation water. Reuse of drainage water is obligatory, but discharge occurs, mainly because of sodium accumulation. The model therefore keeps track of the sodium mass balance in the recirculation water.

For some of the procedures the model makes use of other models, such as KASPRO (De Zwart, 1996) for the simulation of the greenhouse climate.

In GEM, the model is used in the soilless cultivation assessment to calculate the water fluxes and temperatures in the greenhouses. Three-hourly data of the plant water uptake, the sodium related discharge, the filter discharge and the condensation volumes as well as the water uptake –irrigation ratio are provided as output to be used as input for the Substance Emission Model.

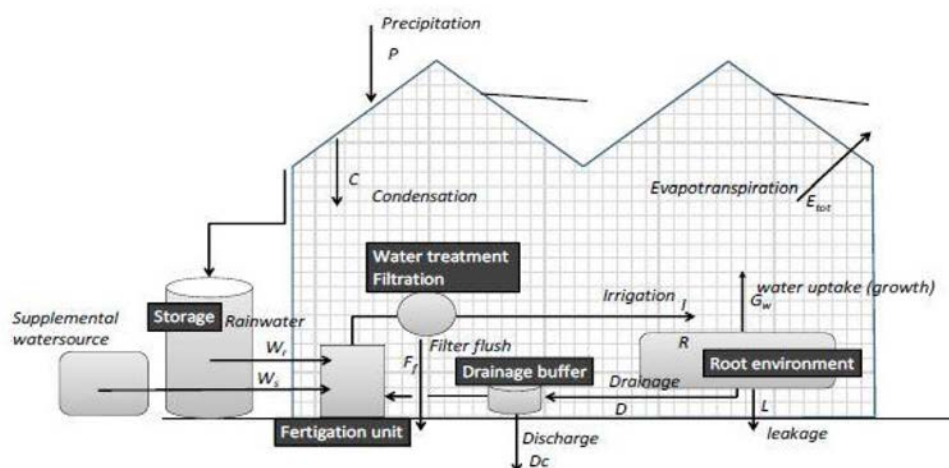


Figure 3.1 Schematic picture of the water fluxes in a greenhouse (Voogt *et al.*, 2012). Harvested rain water and possibly water from supplementary water sources are used for irrigation of crops in the greenhouse. A part of the irrigation water, including possible PPP residues leaves the greenhouse system and enters surface water and/or groundwater.

3.2 Substance Emission Model

The Substance Emission Model (Van der Linden *et al.*, 2015) simulates the fate of PPP in the various water fluxes in the soilless greenhouse system. This model conceptualizes a greenhouse basically as a

number of connected tanks. Water flows from one tank to the other. The model simulates water recirculation based on the water fluxes provided by the WATERSTROMEN model. Within the tanks, PPP is assumed to be ideally mixed, PPP may be degraded, and metabolites may be formed by first order degradation. The uptake of PPP by the crop is simulated with the Briggs formula (Briggs *et al.*, 1982). The model further assumes fixed volumes of the tanks. The volumes are based on typical characteristics of Dutch greenhouse systems. PPP may be applied via the nutrient solution (dripping) or via spraying, fogging or low volume mister. When, PPP is applied via the nutrient solution it enters the recirculation water via a mixing tank. When PPP is applied via spraying, fogging or with a low volume mister it enters the recirculation water via condensation water that is collected and added to the recirculation water and it enters the recirculation water via direct application on flooding tables. Volatilisation and deposition of PPP is considered as well. Sorption to substrate is assumed to be negligible. In case of pot plants, PPP may be sorbed to the substrate (e.g. potting compost) in the pots.

In GEM, the model is used in the soilless cultivation assessment to calculate the PPP fate within the greenhouse. Four crop categories, each different in water requirements and sodium tolerance, are considered. The four crop categories are identified with four representative crops, i.e. tomato, ficus, sweet pepper and rose. For each of the four crop categories, the water fluxes from the WATERSTROMEN model are different and hence, the pesticide concentrations in the recirculation water differ. In case the PPP is applied on pot plants the model allows for sorption to the substrate in the pots. The selected application method defines how PPP enters the simulated system. The hourly discharged volumes and PPP masses for parent and metabolites are given as output, to be used by TOXSWA to calculate the water concentrations in the water body adjacent to the greenhouse. The Substance Emission Model is not available as a standalone application.

3.3 PEARL

PEARL is an acronym for Pesticide Emission Assessment at Regional and Local scales. PEARL (Leistra *et al.*, 2001) is a numerical model that describes the leaching of pesticide to groundwater and, via drainage, to surface water. Water fluxes are simulated with SWAP (Kroes *et al.*, 2008), which is coupled to PEARL. The model is used in Dutch and European pesticide registration procedures. The main processes simulated by SWAP and PEARL are depicted in Fig. 3.2. Recently, PEARL has been extended with a macropore option. For the concepts used to calculate the transport via macropore flow we refer to Tiktak *et al.* (2011).

In GEM, PEARL is used in the groundwater leaching soil-bound cultivation assessment to calculate the groundwater leaching concentration and the 90th percentile annual average concentration in groundwater for the parent and its metabolites. In the surface water exposure assessment for soil-bound cultivation the model is used to calculate the drain emission to the receiving ditch. The hourly drain flow and PPP mass for parents as well as its metabolites in drain flow is provided as output to be used as input for TOXSWA to calculate the concentrations in the ditch adjacent to the greenhouse.

For easy reference, example input files of PEARL are provided in Annex 2 and 3, for groundwater and surface water respectively.

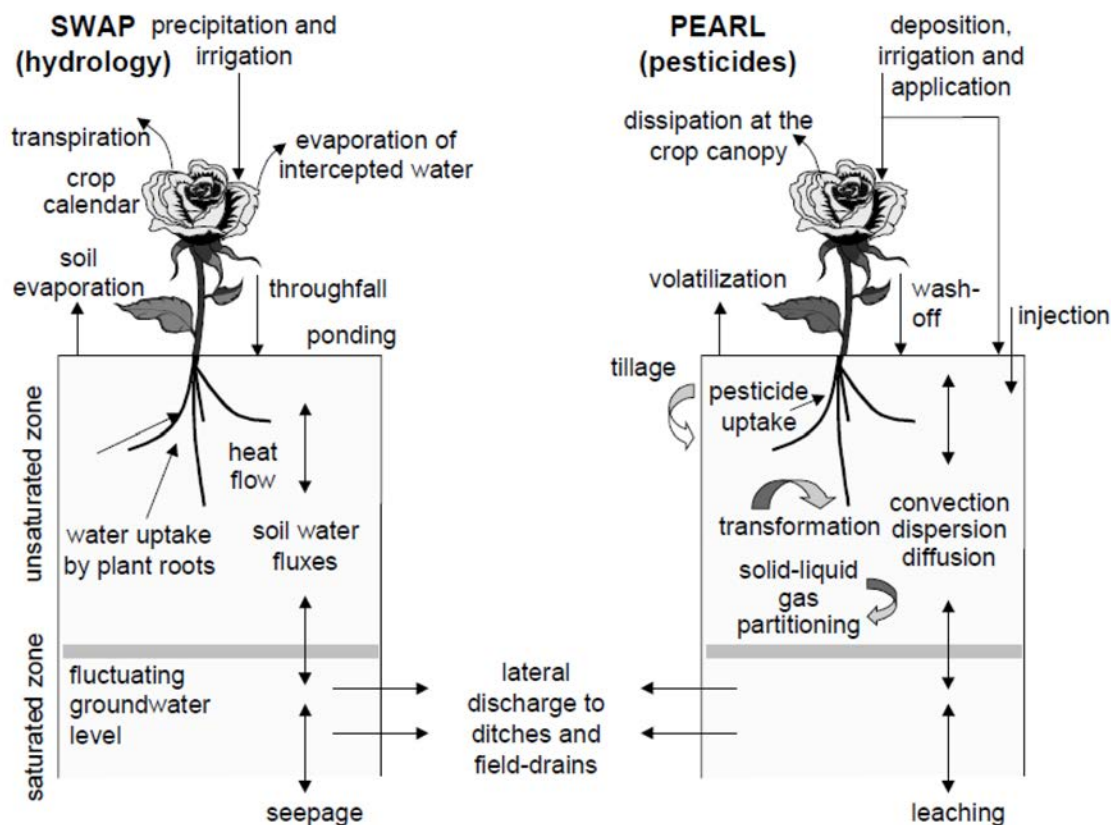


Figure 3.2 Schematic presentation of simulated processes by SWAP and PEARL (source: Tiktak *et al.*, 2000).

3.4 TOXSWA

TOXSWA is the acronym for TOXic substances in Surface WAters. TOXSWA (Adriaanse *et al.*, 1996, Beltman *et al.*, 2014) is a numerical model, simulating pesticide behaviour in a water layer and its underlying sediment at the edge-of-field scale. TOXSWA simulates concentrations of pesticides that may enter the water by spray drift, atmospheric deposition, surface runoff, drainage or leaching through the soil (Figure 3.3). Recently, the model has been extended with an option to simulate the formation and fate of parents and metabolites (Adriaanse *et al.*, 2014). TOXSWA considers transport, degradation, the formation of transformation products, sorption to sediment and suspended solids and volatilisation. The transformation rates cover the combined effect of hydrolysis, photolysis and biodegradation. Transformation and volatilisation are considered to be temperature dependent. Sorption to sediment and suspended solids is described by the Freundlich equation.

For easy reference an example input file of TOXSWA is provided in Annex 4. For those substances with a sorption coefficient (K_{oc}) higher than 1000 L kg^{-1} , the standard sediment segmentation with 14 segments must be refined to reduce the numerical error (Wipfler *et al.*, 2015a). GEM automatically switches to a refined segmentation with 23 segments analogous to Annex 4 in Beltman *et al.* (2014). The example shown in Annex 4 is for a substance with K_{oc} lower than 1000 L kg^{-1} .

The TOXSWA model is used to calculate the water concentrations in the receiving ditch for the surface water assessments. The target percentile annual peak concentration is calculated as well as the TWA concentration for the predefined time window.

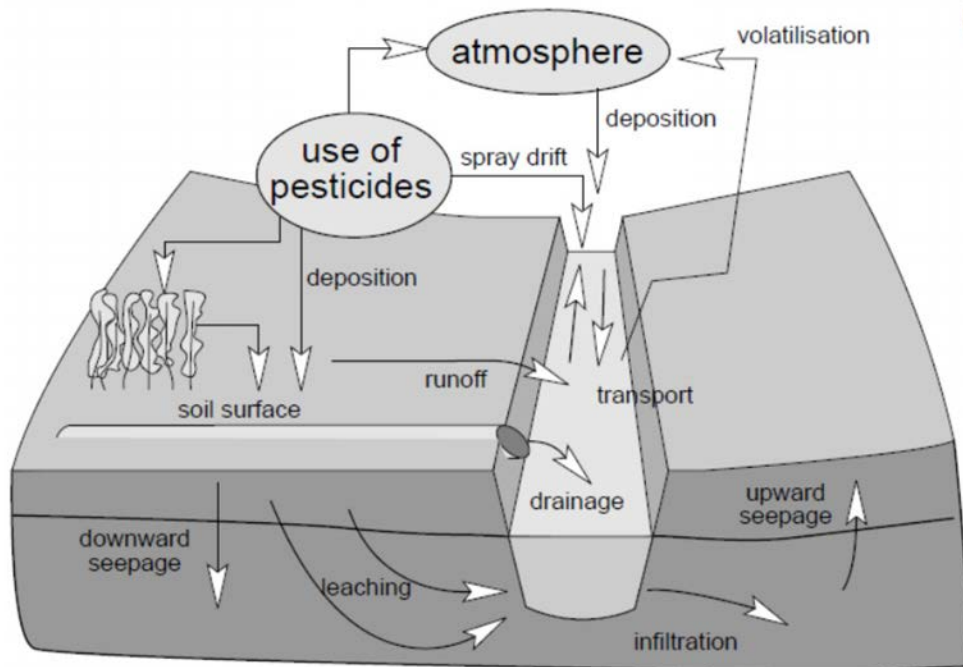


Figure 3.3 Processes and emissions simulated with TOXSWA (source: Beltman et al., 2014).

3.5 Model versions used in GEM

The names, version numbers of the contributing models within GEM are shown in Table 3.1.

Table 3.1

Names and version numbers of the currently used models in GEM.

Module	Version
PEARL	3.2.2
SWAP	3237
SUBSTANCE	1.01
TOXSWA	3.3.3
WATERSTROMEN	1.0

4 Getting started

4.1 Installation

GEM requires the installation of SPIN (Substance Plug IN) for proper functioning. SPIN is used for managing the substance database, and is available on the pesticides website <http://www.pesticidemodels.eu>. Please make sure to install SPIN before running GEM for the first time.

To install GEM run the setup program by right-clicking on the file and selecting 'Run as administrator' (Figure 4.1). Please do not run the program by double-clicking the executable if your user account type is not administrator by default. To install GEM 1.1.1 it is necessary to have (temporary) administrator rights.

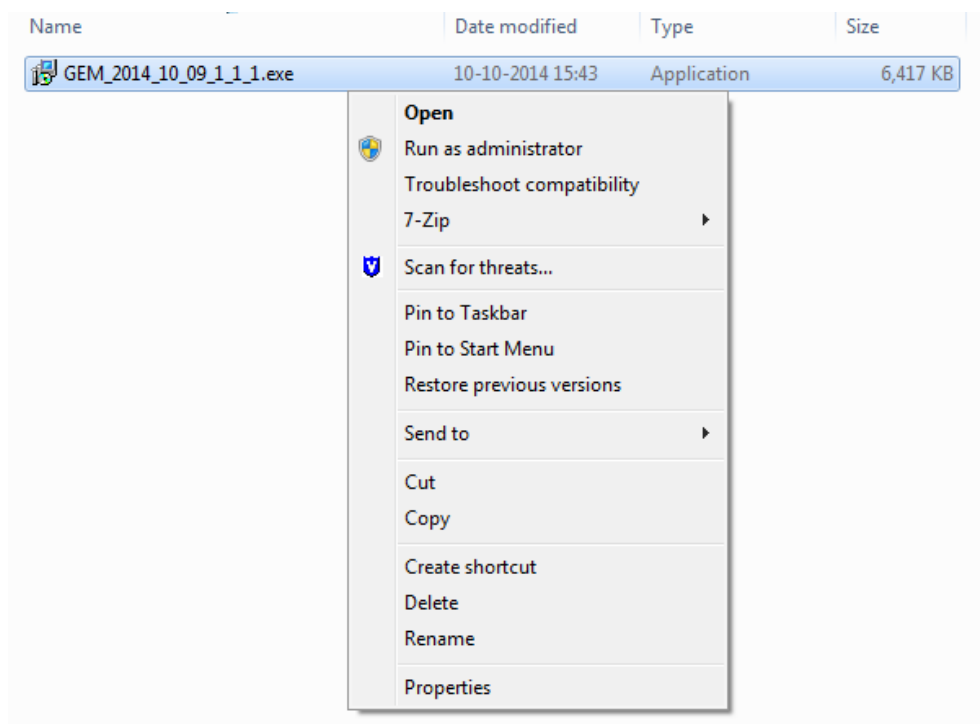


Figure 4.1 For installation of the GEM application select 'Run as administrator'.

By default the program is installed in C:\Program Files\PesticideModels\GEM. This can, however, be changed during installation.

By default the GEM database is installed in a subfolder of the user's personal folder. The exact location differs per user and depends on computer settings and may be governed by company settings. We strongly advise to use a folder on a local drive to guarantee a proper working of GEM.

Note that the GEM instrument and the SPIN application use different settings regarding the decimal mark. SPIN follows the settings of the local computer, whereas GEM expects always a dot as decimal separator!

4.2 Starting up

The GEM program can be started by selecting the program in the 'Start menu' (Figure 4.2). Alternatively, if during installation a short cut icon was created on the desktop, the program can be started by double clicking the icon.

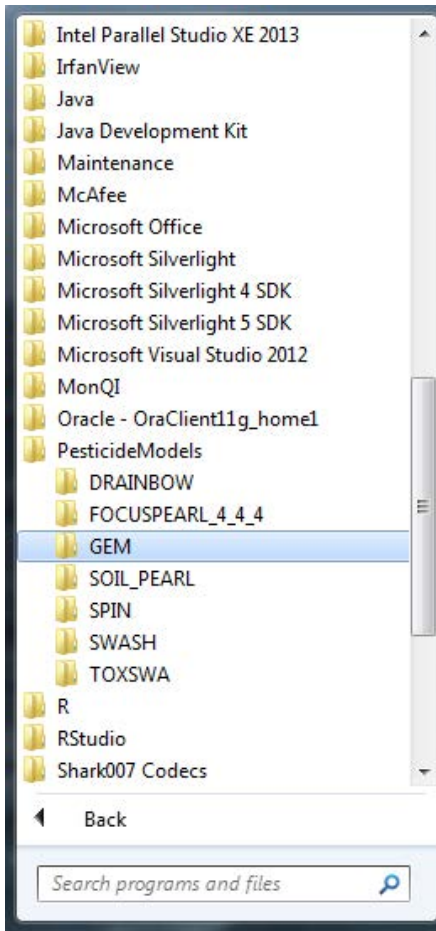


Figure 4.2 Selecting GEM in the Start menu.

4.3 Hard and software requirements

Operating systems:

GEM 1.1.1 has been tested on Windows Vista, Windows 7 and Windows 8.1.

Access rights:

To install GEM 1.1.1 it is necessary to have (temporary) administrator rights.

Preinstalled software:

SPIN version 2.2.

Hard disk memory:

GEM 1.1.1 requires 70 Mb for installation of the application (including the GEM database)

Display:

Monitor with at least 1024x768, at 256 colours. Use as display setting, Font size: Small Fonts.

Processor:

The faster the better.

5 Projects form

5.1 Introduction

When starting GEM, the user is presented with the following view (Figure 5.1).

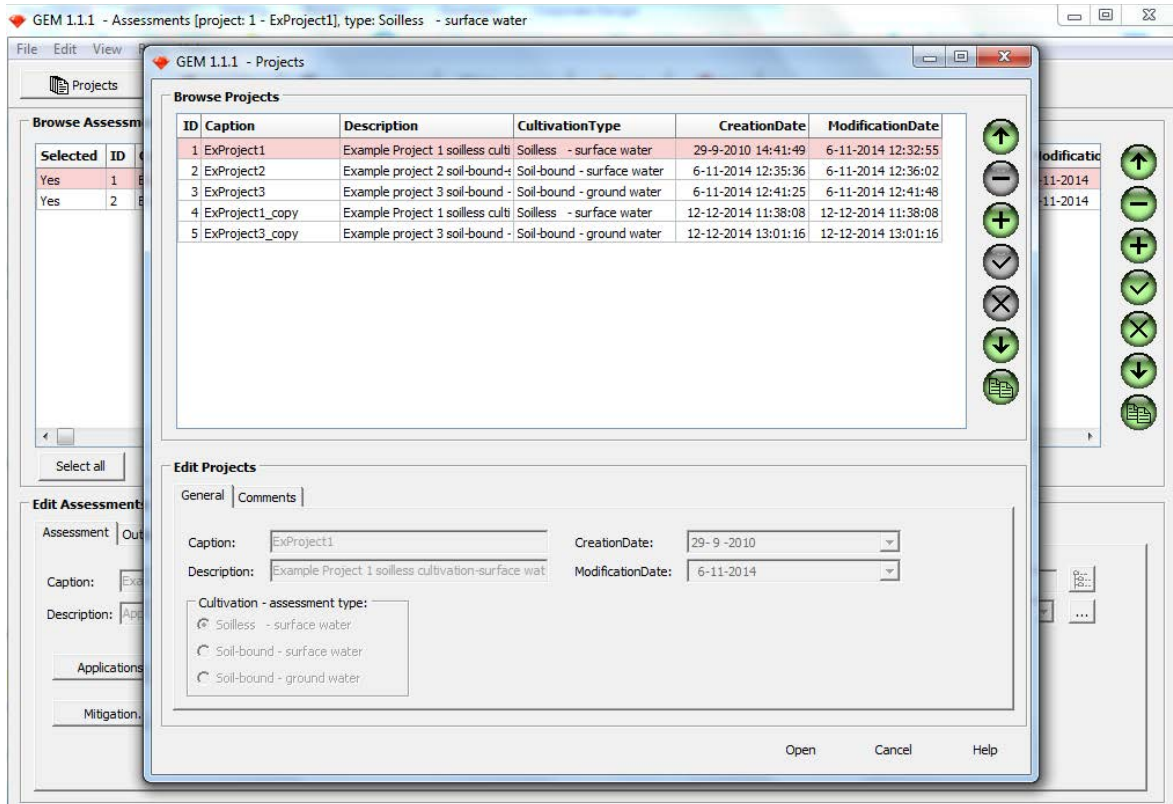


Figure 5.1 The Projects form, the starting point for browsing and editing projects (note that the Assessments form is always shown on the background).

The Projects form is the starting form to define projects. After installation, GEM contains three single projects; there is one example project for each cultivation-assessment type combination. These projects are fixed (i.e. properties cannot be edited), they can only be copied. User-defined projects can be added and will then be shown in the Projects form. The form consists of an upper half, which is used for project management & browsing and the Edit projects section, where the content of the projects can be edited. In the Browse project section, the projects table can be managed by the navigation buttons at the right side of the table as explained Figure 5.2.











-
-  1. Go to the first record (row) in the table
 -  2. Delete the selected record (row)
 -  3. Create a new record (row)
 -  4. Save the changes made by the user
 -  5. Cancel the changes made by the user
 -  6. Go to the last record of the table
 -  7. Copy the selected record

Figure 5.2 Navigation button symbols and their function. Buttons are displayed in green when active (their function is enabled/available) or in grey when inactive, in case the function is presently not allowed or available.

Assessments that belong to a project can be accessed by double clicking on the project name or by selecting the project name and subsequently pressing the 'Open' button in the lower part of the Projects form. The Assessments form, as shown in Figure 6.1, enables the user to define the assessments. The Assessments form is described in Chapter 6.

5.2 Management of stored projects

The user can create a new project from scratch by using the  navigation button. The user is requested to enter a caption (title) and short description of the new project in the 'General' tab of the 'Edit projects'. Additional comments can be entered in the 'Comments' tab. The new project can be saved using the  button, but only if a caption has been supplied. The caption for the new project should be unique.

Alternatively, an existing project can be copied by using the navigation button . The new project will automatically obtain the name of the old project amended by '_copy'. The content of the Description field and Comments field will be inherited (copied) from the original project. The date of creation of the new project will be updated.

5.3 Edit projects

The Edit project section of the Project form (Figure 5.3) enables the user to enter and/or view general information of the selected project, in particular the caption (title) of the project, a description, its date of creation (which cannot be changed), the date it was last changed and comments relating to the project.

5.3.1 Cultivation - assessment type combination

The buttons in the lower left corner of the screen allow selecting the cultivation-assessment type combination of the project. There are three cultivation-assessment type combinations of which only one can be selected in a single project:

- *Soilless - surface water*
- *Soil-bound - surface water*
- *Soil-bound - groundwater*

Soilless – surface water

This cultivation – assessment type combination is applicable to greenhouses where crops are grown on substrate. The endpoint of the assessment is the 50th or 90th percentile of the surface water annual peak concentration as well as the Time Weighted Average Concentration of which the time window is user-defined.

Soil-bound – surface water

This cultivation – assessment type combination is applicable to greenhouses where crops are grown in soils. The endpoint of the assessment is the 90th percentile of the surface water annual peak concentration as well as the Time Weighted Average Concentration of which the time window is user-defined.

Soil-bound – groundwater

This cultivation – assessment type combination is applicable to greenhouses where crops are grown in soils. The endpoint of the assessment is the 90th percentile of the groundwater annually average concentration.

The choice of the cultivation – assessment type combination determines the type of assessments that can be done. Note that if a project has been saved or copied, the selected cultivation – assessment type combination cannot be changed anymore. The user will have to start with a new project!

The screenshot shows a dialog box titled "Edit Projects" with two tabs: "General" and "Comments". The "General" tab is active. It contains the following fields:

- Caption: [Text input field]
- Description: [Text input field]
- CreationDate: [Dropdown menu showing 19-12-2014]
- ModificationDate: [Dropdown menu showing 19-12-2014]

Below these fields is a section titled "Cultivation - assessment type:" with three radio button options:

- Soilless - surface water
- Soil-bound - surface water
- Soil-bound - ground water

At the bottom right of the dialog box are three buttons: "Open", "Cancel", and "Help".

Figure 5.3 *Edit Projects, lower part of the Projects form. Only one of the cultivation – assessment type combinations can be selected. This option is only available when a new project has been opened. After saving the project or copying a new project the cultivation – assessment type combination cannot be changed.*

5.3.2 Buttons

At the lower right part the project form has three buttons:

'Open'

Clicking the 'Open' button will show the Assessments form with assessments that belong to the selected project. The assessment form is discussed in Chapter 6.

'Cancel'

Pressing the 'Cancel' button in the lower part of the Projects form will close the Projects form, and take the user to the Assessments form, where assessments that belong to the selected project are shown and can be accessed.

'Help'

This option links to the user manual.

6 Assessments form

6.1 Introduction

The assessments form enables the user to manage and edit assessments that belong to the selected project. The choice of the Cultivation – assessment type combination in the project form determines which type of assessment can be performed. There is only one possible cultivation – assessment type combination per project.

The Assessments form consists of a header with the GEM version number and the selected project name and cultivation-assessment type combination. Below the header a pull down menu is shown as well as the toolbar, a Browse Assessments section and an Edit Assessments section. These are discussed in the following sections in consecutive order.

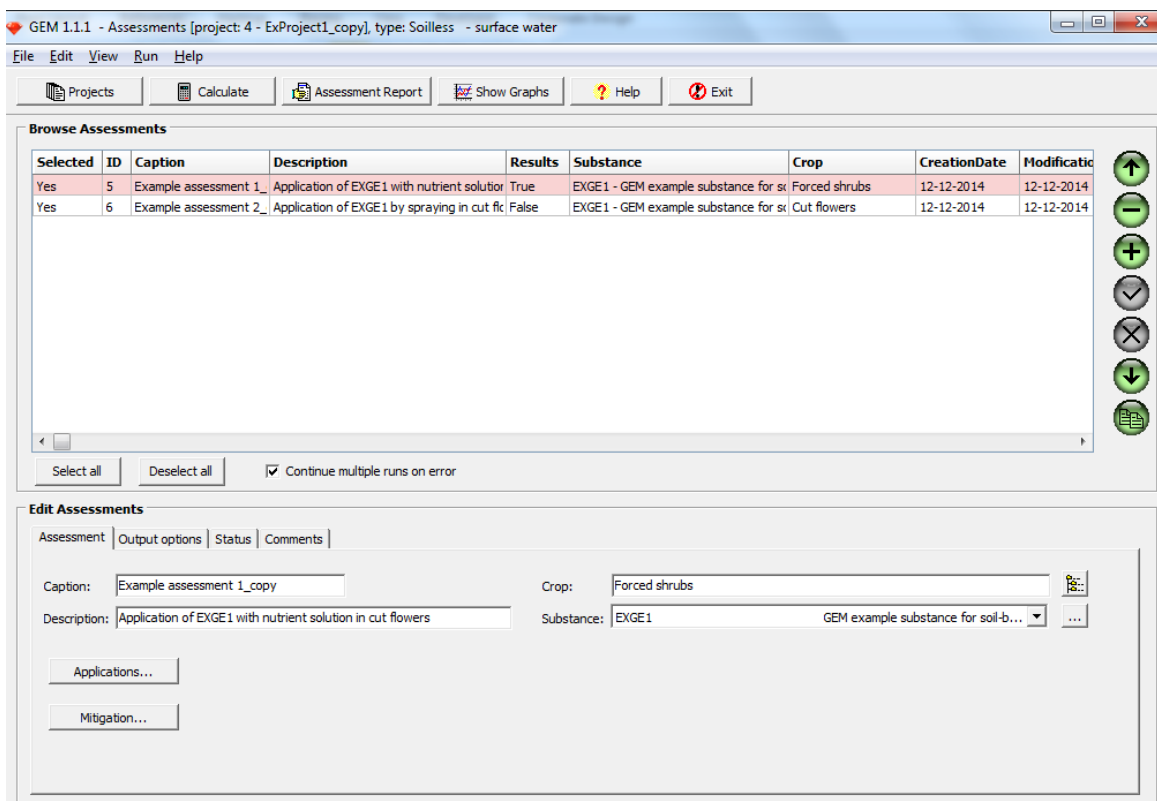


Figure 6.1 The Assessments form, with in the header the project name and cultivation-assessment type combination. The drop down menu is shown below the header, and the toolbar below the drop down menu. In addition there are two sections, a Browse assessment section and an Edit assessment section.

6.2 Assessments form – Menu drop-down options

The assessment form has a number of drop down menu options that can be accessed by clicking the appropriate button in the menu bar ('File', 'Edit', 'View', 'Run' and 'Help').

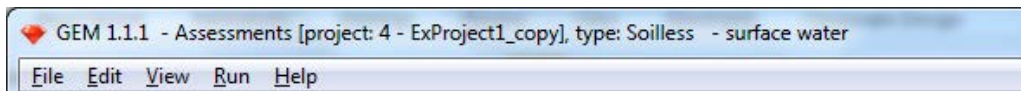



Figure 6.2 The drop-down menu at the top of the Assessments form, just below the header.

6.2.1 File

Via this menu option 'Exit' can be clicked. This option will close GEM and return to the Windows desktop. The user entered information will be stored and will be retained upon starting a new session of GEM.

6.2.2 Edit

Via the menu option 'Edit', the Substance Plug In SPIN is opened. SPIN enables the editing and creation of substances and substance properties. SPIN can alternatively be accessed via the button to the right side of the pick list of substances () on the Assessments tab (Section 6.5). Substance properties can be entered and saved in the Edit Substances section of SPIN. SPIN allows for differentiating between the three cultivation-assessment type combinations, which have each different substance property requirements. SPIN can also be used as a stand-alone application. For further information on SPIN, we refer to Van Kraalingen *et al.* (2013).

6.2.3 View

Input files: This view option allows the user to view the ASCII files generated by GEM as input files for the WATERMODEL, SUBSTANCE-MODEL, PEARL and/or TOXSWA. Input files for each of these programs are presented on a separate tab. The input files are only shown after saving the assessment and only the files of the model relevant for the cultivation – assessment type combination are shown..

Error files: This option allows the user to display error files when available. Errors are also reported to the status tab of the Edit Assessments form.

6.2.4 Run

Continue multiple runs on error: This option is enabled by default. It allows the program to continue its calculations with the next assessment in case of a failed assessment. Setting the option to enabled allows the calculations to continue without an error message being shown. Then, errors can only be observed via display of the output files. This option can alternatively be enabled/disabled via the check box in the Browse substances section.

To allow for inspection of the error messages in case an assessment fails and is aborted, it is recommended to disable the option. Please note that the default 'enabled' state is selected each time GEM is started, regardless of whether the user disabled the option during a previous session of GEM.

6.2.5 Help

About GEM: This option shows information about the model, database and GUI versions used in the GEM version installed, the GUI design and copy rights.

GEM user support: This option provides access to the website, the user manual and related documents.

6.3 Assessments form – Toolbar buttons

Buttons accessible in the Assessments form are shown in Figure 6.3. The functionality that is provided by the buttons is partly redundant with Menu option items.

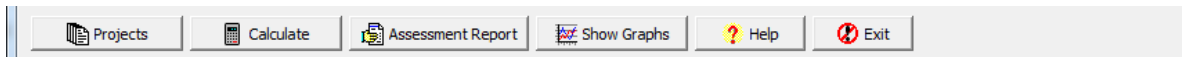


Figure 6.3 *Toolbar buttons of the Assessments form.*

6.3.1 Projects

Opens the Projects screen, giving an overview of existing projects, and enabling the user to add projects or edit existing projects (see Chapter 5).

6.3.2 Calculate

Performs calculations for selected assessments, i.e. the assessments which have a 'Yes' in the 'selected' column. In the example given in Figure 6.4, calculations will be performed for both assessments.

When calculations have finished, a message box pops up. The 'Results' column of assessment switches to 'True', indicating that results have been generated and are available. Prior to the calculations the Results column indicates 'False'.

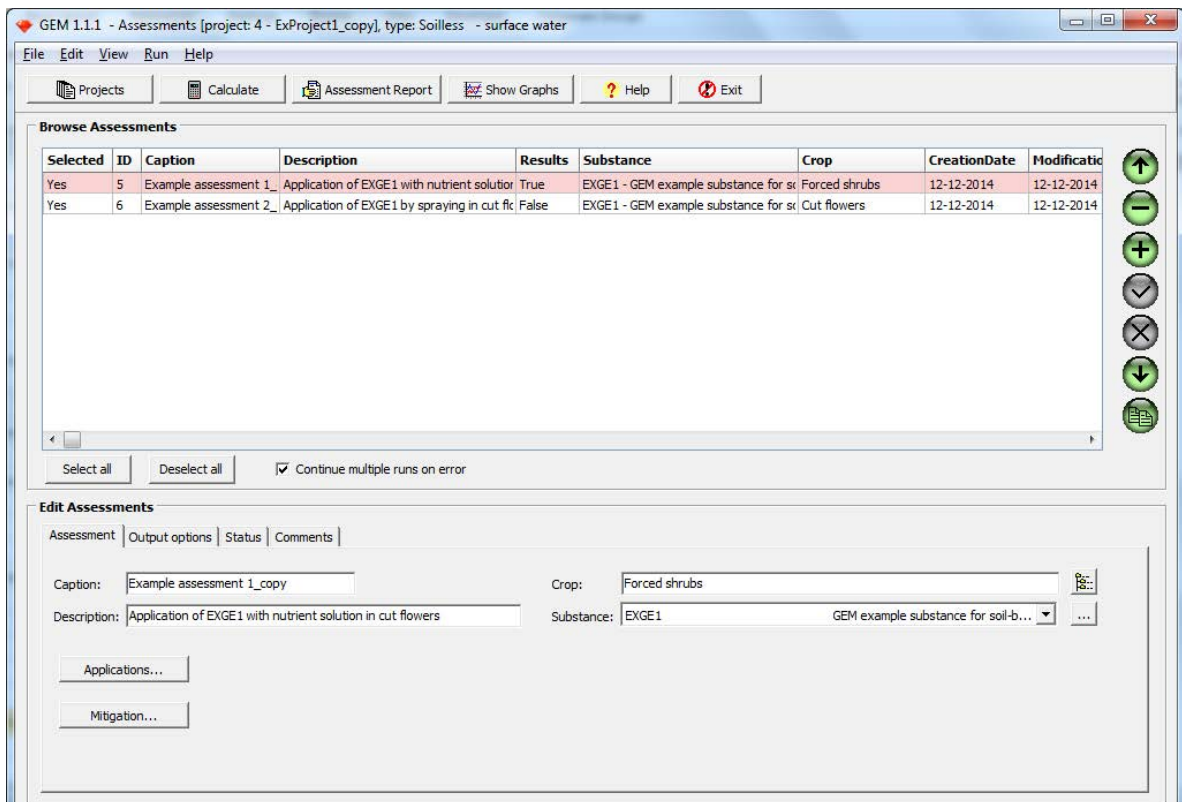


Figure 6.4 *The Assessments screen indicating that calculations are enabled for Assessment ID 5 and 6, as indicated by 'Yes' in the leftmost 'Selected' column). Only for assessment 5 the calculations have been done and results are available (as indicated by 'True' in the 'Results' column).*

6.3.3 Assessment Report

Pressing the 'Assessment Report' button in the Tool bar will cause the generation of a report summarizing the calculation results of the selected assessment. Results are presented in a web browser window, which can be printed while using the standard print options of your web browser. The

report merges the main results of summary reports of the SUBSTANCE-MODEL, PEARL and TOXSWA depending on the cultivation – assessment type combination selected. Trying to generate an assessment report for which no results are available will result in an error message, indicating that no results are (yet) available for this assessment.

The report consists of a header with general assessment information, the model versions that are used by GEM, then for each of the applied models a summary of input and results of the calculations. Summary results for the calculation of peak concentrations and time weighted average (TWA) exposure concentrations are given at the end of the report. An example of a complete report for each of the cultivation - assessment type combinations is given in Annex 5.

6.3.4 Show Graphs

The 'Show graphs' button opens a selection screen enabling the user to select four types of graphs for the parent, and if relevant also for the metabolites (Figure 6.5). This option is only valid for surface water exposure assessments; the groundwater assessment does not allow for showing graphs. To enable the display of graphs the output option 'All needed for viewing graphical output with GUI' must be selected before calculating the assessment. This option is shown on the Output tab, which is discussed in Section 6.5.2. Also the time-windows for the Time Weighted Average concentrations can be defined on the Output tab.

The optional graphs are:

- a. Discharged daily mass to ditch for the 50th or 90th percentile year (Figure 6.6). This figure is only available for soilless cultivation. The value of the percentile depends on the selection of the user. The year nearest to the selected percentile is shown. Since the calculations are done over a period of seven years, the 50th percentile will be the fourth in line of the ranked annual peak concentrations and the 90th percentile will be the seventh of the ranked annual peak concentrations.
- b. Average substance concentration for the 50th or 90th percentile year (Figure 6.7). The water concentration is plotted at the end of each hour, averaged over 100 m of ditch. The year nearest to the selected percentile is shown. Since the calculations are done over a period of seven years, the 50th percentile will be the fourth in line of the ranked annual peak concentrations and the 90th percentile will be the seventh of the ranked annual peak concentrations.
- c. Averaged substance concentration over the entire simulation period (Figure 6.8). The water concentration is plotted at the end of each hour, averaged over 100 m length of ditch.
- d. TWA (Figure 6.9). The Time Weighted Averaged surface water concentration is plotted for the selected year and over the time window as provided by the user. Also the average concentration is plotted. Both concentrations are plotted at the end of each hour and averaged over 100 m length of ditch.

If the user has selected an assessment for which no calculation results are available, and tries to generate graphs anyway, he/she will be informed that the necessary data is not available or invalid.

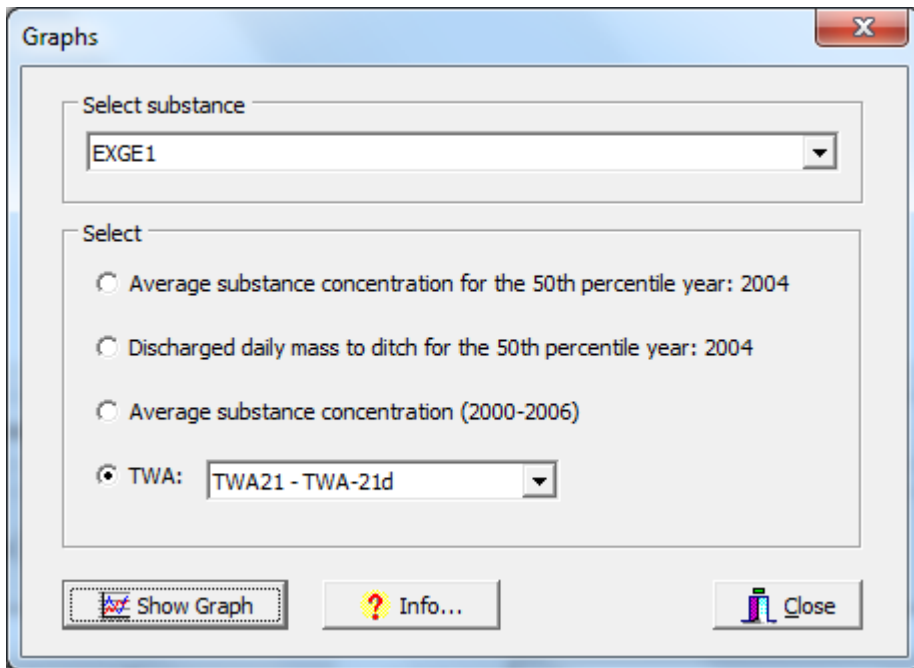


Figure 6.5 Graphs form accessible by pressing the button 'Show graphs' on the Assessment form.

Pressing the 'Info' button on the Graphs screen will generate a text window giving some additional information of what type of graph may be produced, whereas pressing the 'Close' button will take the user back to the Assessments form.

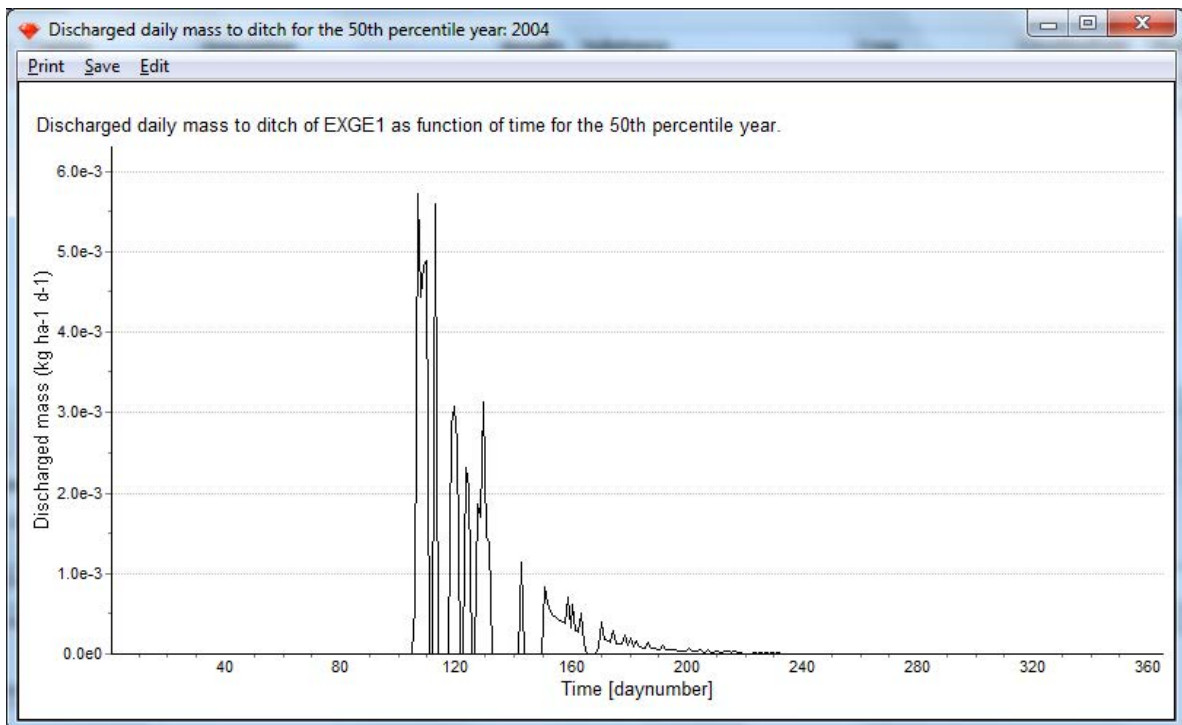


Figure 6.6 Results when selecting 'Show Graphs' for an assessment (option 'Discharged daily mass to ditch for the 50th or 90th percentile year').

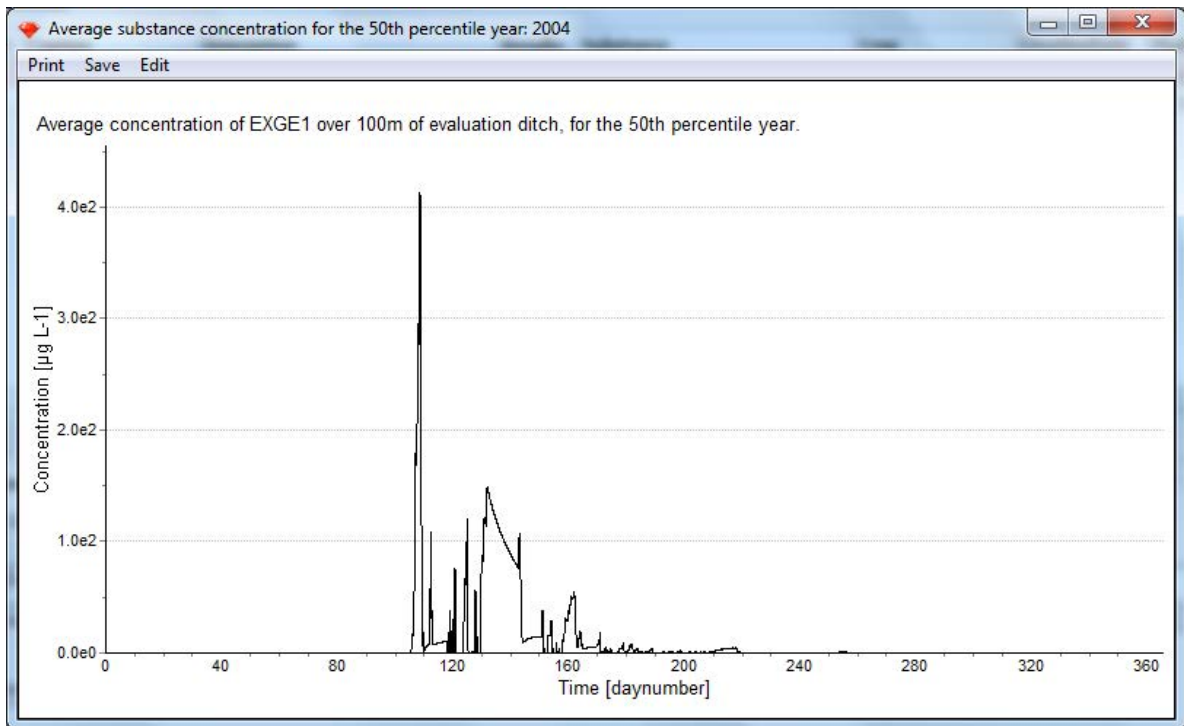


Figure 6.7 Results when selecting 'Show Graphs' for an assessment (option 'Average substance concentration for the 50th or 90th percentile year').

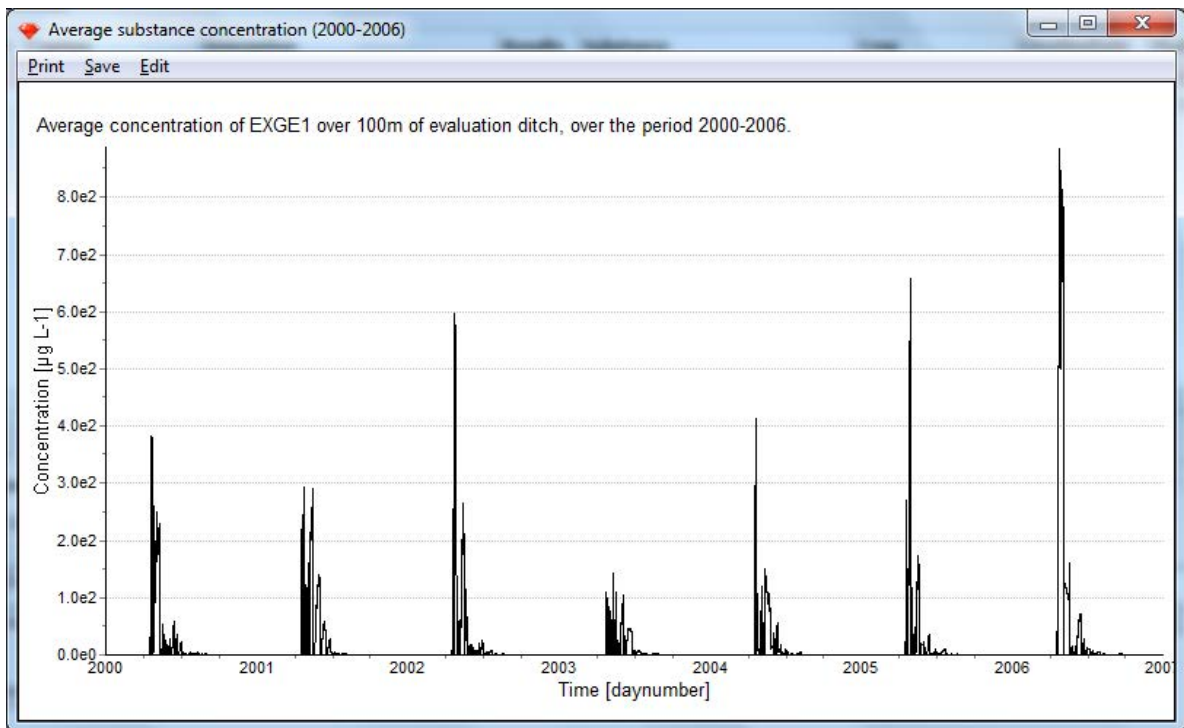


Figure 6.8 Results when selecting 'Show Graphs' for an assessment (option 'Average substance concentration (2000-2006)').

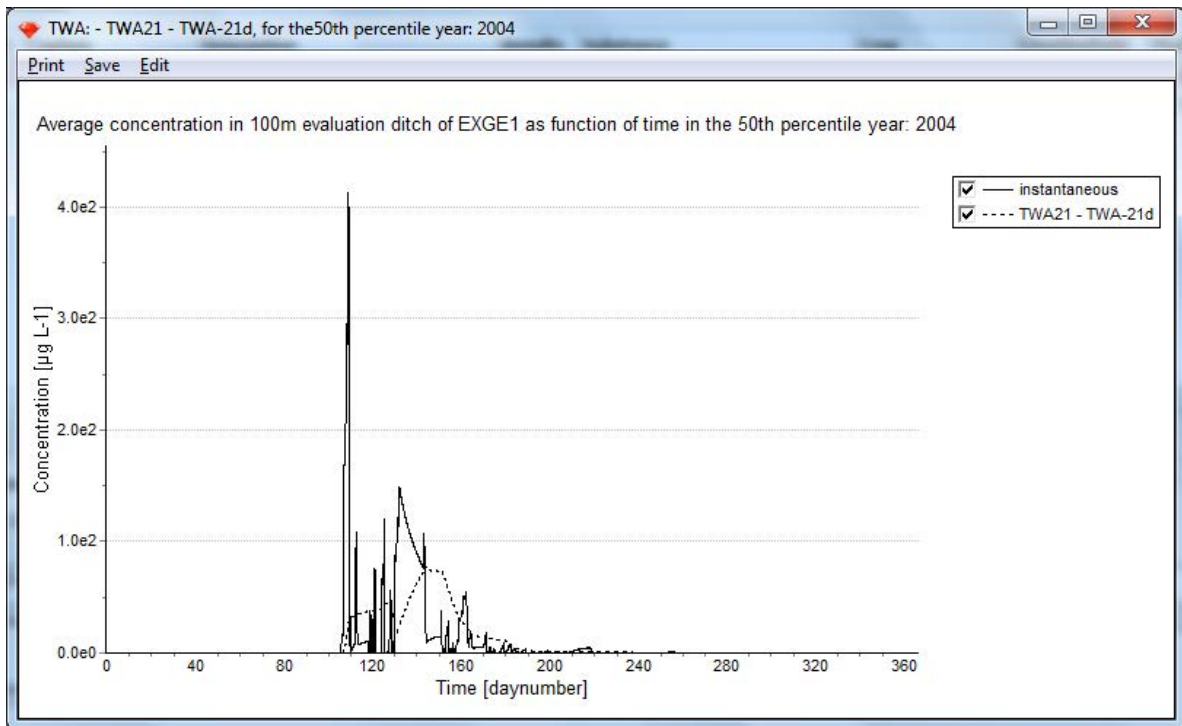


Figure 6.9 Results when selecting 'Show Graphs' for an assessment (option 'TWA:').

The three buttons: Print, Save and Edit on the screen showing the graph allow the user to respectively Print, Save or edit the graph; Charting Library TeeChart is used to chart the output of the model. The working of the TeeChart Print Preview (summoned by button Print) and Export Dialog screen (summoned by button Edit) is self-explaining and not further discussed here. Editing graphs is not desirable in a regulatory context and therefore not discussed in this manual. However via the Help button help files on TeeChart can be started.

6.3.5 Help

This option provides access to the website, the user manual and related documents.

6.3.6 Exit

Leave GEM and return to the Windows desktop. The user entered information has already been stored at this point, and will therefore be retained upon starting a new session of GEM.

6.4 Assessments form – Browse assessments

The Browse Assessments section can be found right below the toolbar and above the Edit Assessments section. In this section, data can be viewed or copied but not changed. The assessments of the selected project are listed and can be browsed by using the navigation buttons at the right-hand side of the screen. New assessments can be created by using the navigation buttons. The function of the navigation buttons is similar to those in the Project form as explained in 5.1. and shown in Figure 5.2. Assessments can be selected for calculation by double clicking the assessment.

6.4.1 Select all / Deselect all

Below the list of assessments the buttons Select all and Deselect all are shown. These buttons allow to select or deselect the entire list of assessments as shown in the Browse assessment form. Note that it is possible to run multiple assessments within one project.

6.4.2 Continue multiple run on errors

The check box Continue multiple run on errors allows the program to continue its calculations with the next assessment in case of a failed assessment. Setting the option to 'enabled' allows the calculations to continue without an error message being shown. Errors can only be observed via display of the output files. The option is enabled by default. This option can alternatively be accessed via the drop down menu (Section 6.2).

To allow for inspection of the error messages in case an assessment fails and is aborted, it is recommended to disable this option. Please note that the default 'enabled' state is selected each time GEM is started, regardless of whether the user disabled the option during a previous session of GEM.

6.5 Assessments form – Edit Assessments

The Edit assessments section is located in the lower half of the Assessments form (Figure 6.10). Four different tab sheets can be selected, being the Assessment tab, the Output tab, the Status tab and the Comments tab. Note that if one of the item changes in one of the tabs, the Results are set to False and the assessment should be recalculated. The four tab sheets are described in the next sections.

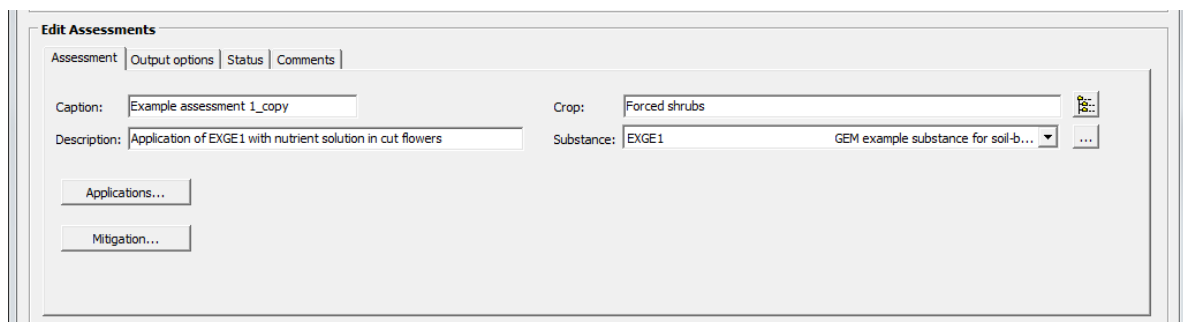


The screenshot shows the 'Edit Assessments' window with the 'Assessment' tab selected. The window has a title bar 'Edit Assessments' and four tabs: 'Assessment', 'Output options', 'Status', and 'Comments'. The 'Assessment' tab contains several input fields: 'Caption' with the text 'Example assessment 1_copy', 'Description' with 'Application of EXGE1 with nutrient solution in cut flowers', 'Crop' with 'Forced shrubs', and 'Substance' with 'EXGE1'. There are also two buttons: 'Applications...' and 'Mitigation...'. The 'Substance' field has a dropdown menu showing 'GEM example substance for soil-b...' and a small icon to its right.

Figure 6.10 Edit assessments – tab sheet Assessment.

6.5.1 Assessment Tab

Caption and Description: The user may provide a Caption of the assessment, and optionally a Description.

Crop: A crop can be selected by pressing the button at the right side of the crop input field, which opens up the list of crops. Crops are clustered according to the Dutch DTG list into related groups. The crops underlying clusters can be made visible by pressing the  navigation button next to the name of the crop cluster. Only one single crop can be selected (Figure 6.11). For soilless cultivation only crops can be selected that are grown soilless and for soil-bound cultivation only crops can be selected that are grown soil-bound. The lists of crops are given in Annex 1. Crops not relevant for the selected cultivation type are indicated with .

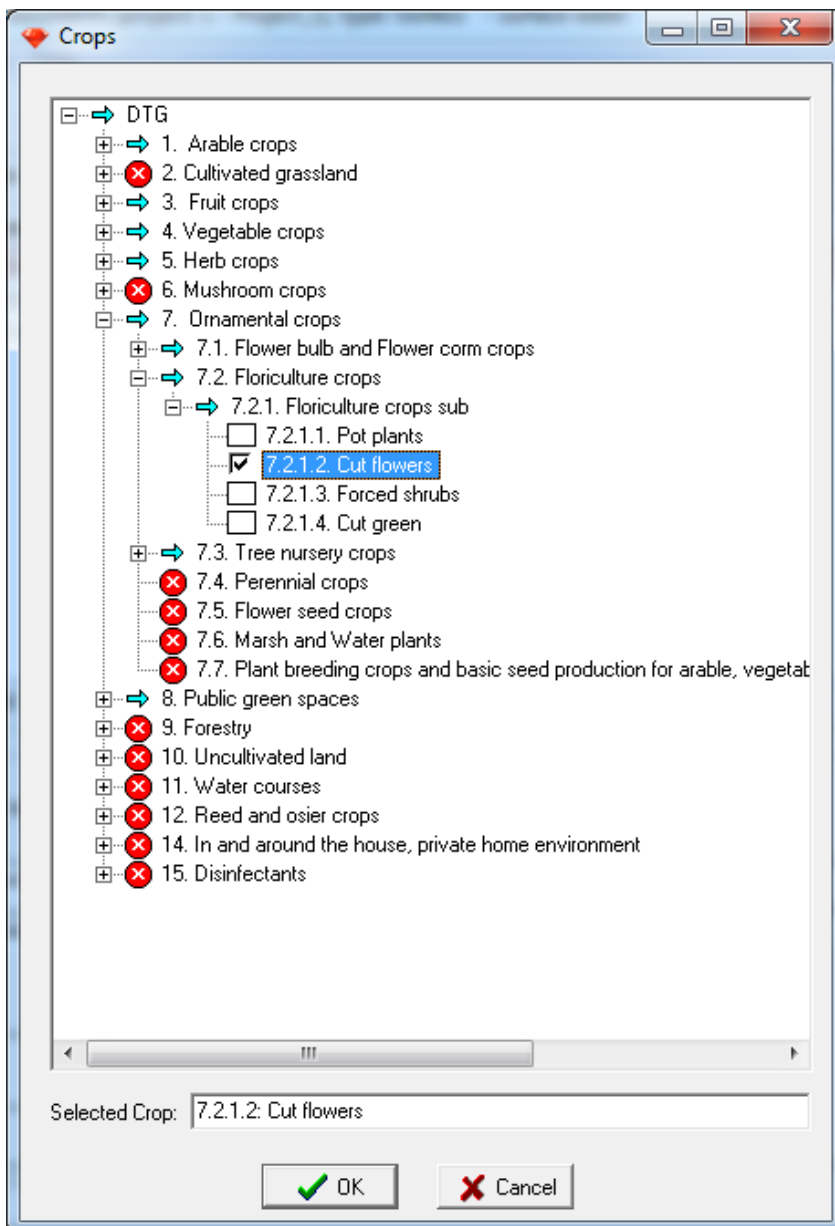


Figure 6.11 Edit assessments – tab sheet Assessment – Crop selection from the DTG list.

Substance: A substance to be used in the assessment can be selected by clicking the Substance list box button. The substance is indicated 'incomplete' if not all required properties are available. For editing of the substance properties or adding a new substance, press the button to the right of the substance pick list to open the Substance PlugIn SPIN. The required substance properties may differ per assessment-cultivation type combination. In SPIN also metabolite formation schemes can be entered and modified to define the relation between the parent and the metabolites formed in the different environmental compartments. For further explanation of SPIN we refer to Van Kraalingen *et al.* (2013).

SPIN provides information in case the substance properties are incomplete (see Figure 6.12). Note however that this information is only provided in the case the option 'Continue multiple runs on error' is disabled. In case the option 'Continue multiple runs on error' is enabled, Figure 6.12 is not shown, but also there is no error message given in the box 'ErrorMessage' on the tab 'Status'.

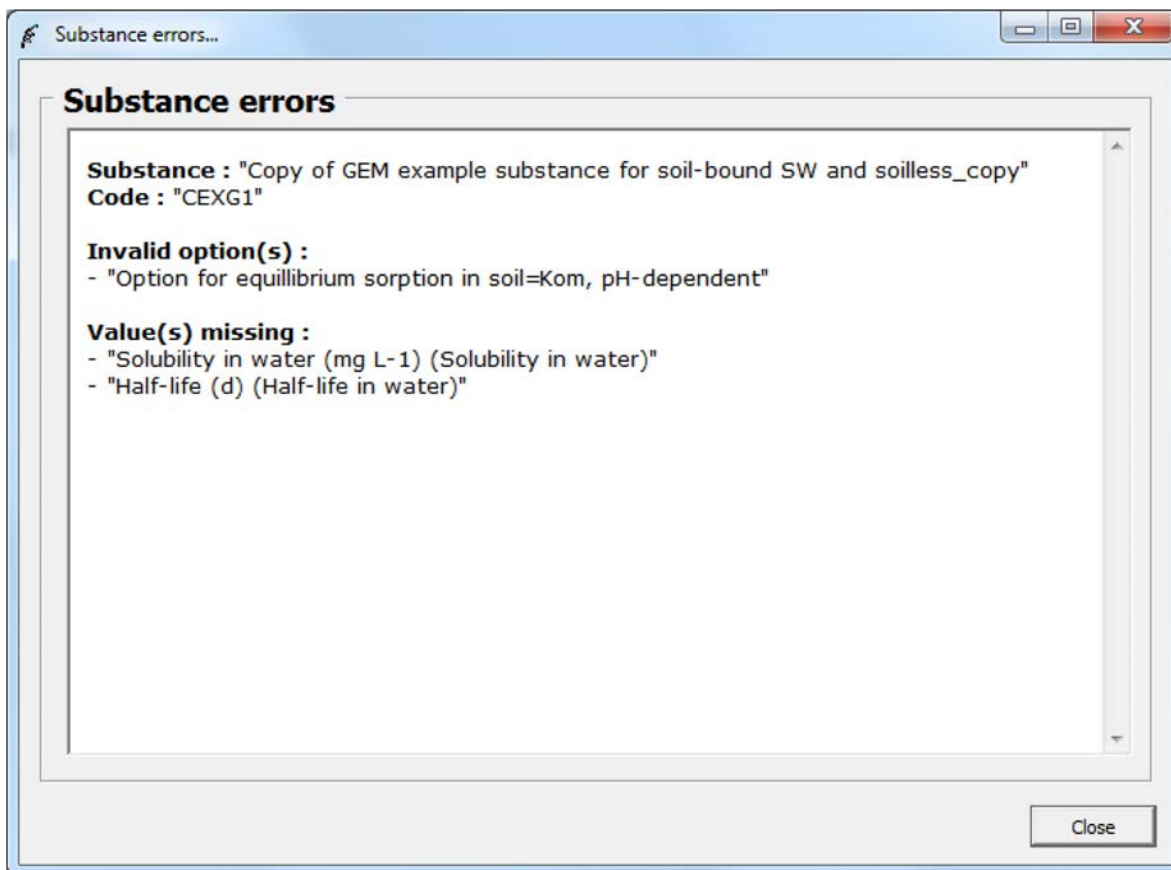


Figure 6.12 Incomplete substance properties notification. This notification is only shown when the option 'Continue multiple runs on error' is disabled.

Applications button: After clicking the Applications button the Applications form will pop up (Figure 6.13). In this form applications can be modified or added, analogous to the handling of Projects and Assessments. The user must specify the application type, the applied dose and the application date for each application, which are applied annually.

Application types that can be selected depend on the selected Cultivation - assessment type. Options are listed in Table 6.1. The application parameter Depth [m] is only relevant for the application types 'Incorporation' and 'Injection' and application parameter Fraction intercepted [-] is only relevant for the application type 'To the crop canopy'. If the Application parameter is not relevant for the selected application type the field remains grey and cannot be selected.

Table 6.1

Selectable Application types per Cultivation - Assessment type and required additional information.

Application type	Soilless-surface water	Soil-bound -surface water	Soil-bound - groundwater	Additional information
With nutrient solution	X			-
Spraying	X			-
Fogging	X			-
Low volume mister	X			-
To the crop canopy		X	X	Fraction intercepted (-)
To the soil surface		X	X	-
Incorporation		X	X	Depth (m)
Injection		X	X	Depth (m)

Browse Applications

Nr.	ApplicationType /	ApplicationDate	Dosage	Applications parameter
1	Incorporation	01-Apr	0.3	0.05
2	Injection	07-Apr	0.75	0.1
3	To the soil surface	25-Apr	0.25	
4	To the crop canopy	01-Jun	1	0.35

Edit Applications

ApplicationType:

Application date: /

Dosage [kg.ha-1]:

Application parameter:

Depth [m]:

Fraction intercepted [-]:

Close

Figure 6.13 Applications form. The application types shown are valid for soil – bound cultivation. The application parameters Depth [m] and Fraction intercepted [-] are only relevant for the application types 'To the crop canopy', 'Incorporation' and 'Injection'. If the Application parameter is not relevant for the selected application type the field remains grey and cannot be selected.

Mitigation button: After clicking the Mitigation button the Mitigation form will pop up (6-14). The function is only available for projects with Soilless cultivation and offers the user to specify an end-of-pipe removal factor. This factor quantifies the optional impact of water treatment on substance concentrations in discharged water. Mitigation records can be modified or added, analogously to the handling of Projects and Assessments. The removal factor can be specified for a substance and, if applicable, in separate records for its metabolites. The removal factor may have a different value per assessment as well as for parent and metabolites.

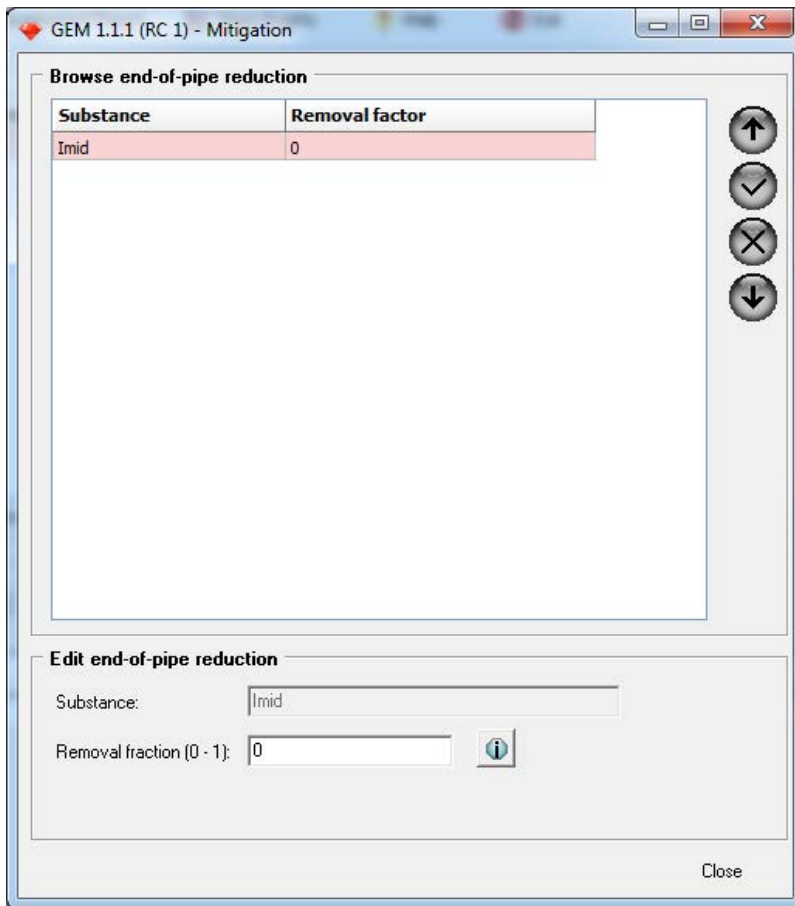


Figure 6.14 Mitigation form (Soilless cultivation only).

6.5.2 Output options Tab

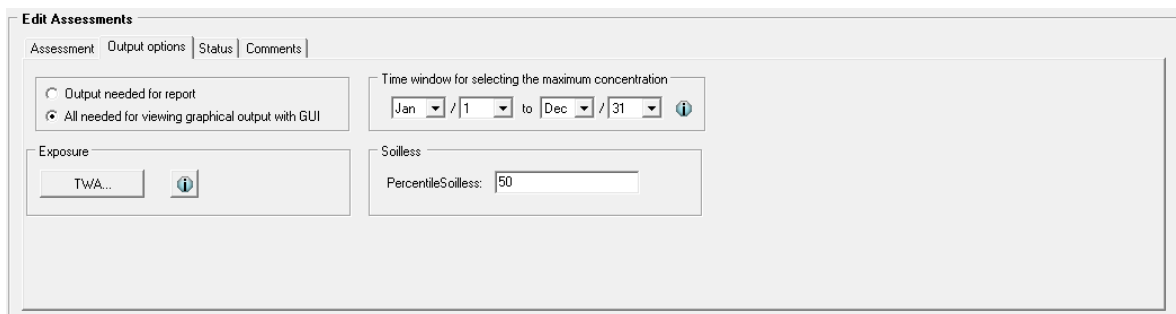


Figure 6.15 Edit assessments – tab sheet Output options.

The tab sheet Output enables to specify the required output. The user may select to generate 'Output needed for report' consisting of basic output in text format, or alternatively may select to generate 'All needed for viewing graphical output with GUI' which generates not only the basic output in text format, but allows the user to generate graphical output within GEM. Note that when selecting the graphical output option, the required storage per substance is approx. 12 MB.

For soilless cultivation either 50th percentile or 90th percentile concentration must selected as target endpoint of the simulation before starting the calculations.

The Time window for selecting the maximum concentration allows the user to limit the period in a year from which the maximum concentration is selected. This feature is useful if or when there are ecological or eco-toxicological reasons for assessing the risks in a specific part of the year only (when

e.g. the substance is only toxic to the organism during their reproductive stage). This option is available only for the surface water exposure assessments.

TWA button: The software will by default calculate and report Time Weighted Average (TWA) concentrations calculated over periods of 7 days (TWA7) and 21 days (TWA21). The user can specify one or more additional TWA entries in the TWA form and GEM will provide additional output for these selected TWA entries (Figure 6.16). This option is only valid for surface water exposure scenarios. The number of TWA entries and the selected time window per entry are assessment specific properties; they have to be defined per assessment.

6.5.3 Status Tab

The tab sheet 'Status' shows the status of the assessment, it is not intended for editing (Figure 6.17). The Status tab gives some assessment specific information also given in the upper part of the Browse Assessments screen (i.e. columns: Selected, Creation, Modification, Results, Error message). For the assessment selected, the Status tab provides information on whether the assessment has been selected for calculations, i.e. will output be generated when calculations are performed, and whether results are available. Furthermore, in case the calculation of the selected assessments was aborted due to an error, the error message will appear in the ErrorMessage box on the right-hand side of the screen.

6.5.4 Comments Tab

The tab sheet 'Comments' offers the possibility to the user to add comments to an assessment. This tab opens a memo box where the user can note comments that will be stored with the assessment data. The results become invalid if the comment in the comment box has been changed.

The screenshot shows the 'GEM 1.1.1 - TWA' window. It features two main sections: 'Browse exposure periods' and 'Edit exposure period'. The 'Browse exposure periods' section contains two tables. The first table, 'Defaults:', lists TWA7 and TWA21 with their respective durations and relevant periods. The second table, 'Additional (max 8 + 2):', shows a single row with '<not available>' for all fields. To the right of the tables are several control buttons: an up arrow, a minus sign, a plus sign, a checkmark, an 'X', a down arrow, and a printer icon. The 'Edit exposure period' section at the bottom has input fields for 'Name:' and 'Duration [d]:', and a 'Relevant period' section with 'Start:' and 'End:' dropdown menus. The 'Start:' dropdown is set to 'Jan' and '1', and the 'End:' dropdown is set to 'Jan' and '31'. A 'Close' button is located at the bottom right of the window.

Name	Duration [d]	Start Relevant Period	End Relevant Period
TWA7	7	01-Jan	31-Dec
TWA21	21	01-Jan	31-Dec

Name	Duration [d]	Start Relevant Period	End Relevant Period
<not available>	<not available>	<not available>	<not available>

Figure 6.16 TWA form.

Edit Assessments

Assessment | Output options | **Status** | Comments

Selected for execution:

CreationDate: 6-3-2014

ModificationDate: 20-10-2014

Results: available

ErrorMessage:

Figure 6.17 Edit assessments – tab sheet Status.

7 Additional guidance to the user

7.1 Substance properties in greenhouse soils (soil-bound cultivation)

For the soil-bound cultivated crops it is recommended to carry out degradation experiments in greenhouse soils to derive the substance half-lives. Degradation is likely to be lower in greenhouse soils after sterilisation of these soils. As a result, using half-lives from open field soils in combination with the newly developed scenario is questionable. See for further details Wipfler *et al.* (2015a).

For suggestions for the other substance properties that can be used in the soil-bound crop cultivation assessments, we refer to Wipfler *et al.* (2015a), Annex 4. The main values are listed below:

- E_a for degradation in soil: 65.4 kJ/mol (EFSA 2007)
- Factor B describing moisture dependency of degradation in soil: 0.7 (FOCUS 2000)
- E_a for hydrolysis in surface water: 75 kJ/mol (Deneer *et al.*, 2010)
- Wash-off factor: 0.1 mm⁻¹ conservative value for leaching and drainage assessments, based on EFSA (2012)
- Depth dependency of degradation in soil as proposed by FOCUS (2000)
- Uptake factor for plants: 0.0 (FOCUS 2000)
- Molar enthalpy of vaporisation: 95 kJ/mol (FOCUS 2000)
- Molar enthalpy of dissolution: 27 kJ/mol (FOCUS 2000)
- Molar enthalpy of sorption: 0 kJ/mol (FOCUS 2000)
- Reference diffusion coefficient in water: $0.43 \times 10^{-4} \text{ m}^2 \text{ d}^{-1}$ (FOCUS 2000)
- Reference diffusion coefficient in air: $0.43 \text{ m}^2 \text{ d}^{-1}$ (FOCUS 2000)
- Reference temperatures for diffusion, vapour pressure, water solubility, sorption, transformation rates in soil and water: 20 °C
- Half-life for dissipation from plant surfaces: 10 d (EFSA, 2012). DT50 due to penetration: 1000 d
- Molar enthalpy of transformation in surface water and sediment: 65.4 kJ/mol.

7.2 Substance properties in soilless cultivation

There is no prescribed guidance for the derivation of substance degradation properties in soilless cultivation. As degradation rates in recirculation water are generally not available, the user may consider to use the degradation rate due to hydrolysis. Furthermore the following additional properties may be used in the calculations (see also Wipfler *et al.* (2015b):

- Half-life on crop: 10 d
- Half-life on floor: 100 d
- Molar enthalpy of transformation in recirculation water: 65.4 kJ/mol
- Molar enthalpy of transformation in air: 45 kJ/mol

Note that for the soilless cultivation assessment, Briggs *et al.* (1982) is used for calculating the plant uptake, whereas for soil-bound cultivation the plant uptake factor is used. The application of the Briggs formula requires that the octanol-water partition coefficient has been filled.

7.3 pH dependent sorption

pH dependent sorption cannot be simulated with the current version of GEM. The TOXSWA model does not allow for pH dependent sorption, neither does the Substance Emission Model. PEARL does allow for pH dependency however, the pH of the various soil layers has not been defined.

7.4 Greenhouse discharged volumes and mass

For advanced users the calculated discharge water volumes and mass towards the ditch are stored in files which can be accessed via the directory structure as shown in Section 2.3.

For the surface water exposure assessment for soilless cultivation the file can be found within the folder SUBSTANCE. The file has the extension g2t (see example in Figure 7.1). The files provides the hourly water fluxes and mass fluxes per m² of cultivated land for the parent and metabolites.

```

*-----
* Results from the Substance Emission model (c) Alterra, WUR Greenhouse Horticulture and RIVM
* Substance Emission kernel version : v1.1.1
* SUBSTANCE EMISSION MODEL created on : 06-Nov-2014
*
* Working directory      : D:\UserData\GEM\Projects\1\10\SUBSTANCE
* Run ID                 : 10
* Input file generated on : 02-Mar-2015 12:07:32
*-----
* application type: application with nutrient solution
*
* Number of substances: 1
* Parent substance:    EXGE1
* Metabolite substances:
*
* NumApp      7
* Number      Start of application      End of application      Dosage
* 1           15-Apr-2000 00:00:00      15-Apr-2000 02:00:00   0.8400
* 2           15-Apr-2001 00:00:00      15-Apr-2001 02:00:00   0.8400
* 3           15-Apr-2002 00:00:00      15-Apr-2002 02:00:00   0.8400
* 4           15-Apr-2003 00:00:00      15-Apr-2003 02:00:00   0.8400
* 5           15-Apr-2004 00:00:00      15-Apr-2004 02:00:00   0.8400
* 6           15-Apr-2005 00:00:00      15-Apr-2005 02:00:00   0.8400
* 7           15-Apr-2006 00:00:00      15-Apr-2006 02:00:00   0.8400
*
* Units:
* VolOut2SurWat (m3 hr-1 m-2)
* MasOut2SurWat_EXGE1 (g hr-1 m-2)
*
* Legend to columns:
* Time      Date      Time      VolOut2SurWat      MasOut2SurWat_EXGE1
* 0.021     01-Jan-2000-00:30 0.0000E+00 0.0000E+00
* 0.062     01-Jan-2000-01:30 0.0000E+00 0.0000E+00
* 0.104     01-Jan-2000-02:30 0.0000E+00 0.0000E+00
* 0.146     01-Jan-2000-03:30 0.0000E+00 0.0000E+00
* 0.188     01-Jan-2000-04:30 0.0000E+00 0.0000E+00
* 0.229     01-Jan-2000-05:30 0.0000E+00 0.0000E+00
* 0.271     01-Jan-2000-06:30 0.0000E+00 0.0000E+00
* 0.312     01-Jan-2000-07:30 0.0000E+00 0.0000E+00
* 0.354     01-Jan-2000-08:30 0.0000E+00 0.0000E+00
* 0.396     01-Jan-2000-09:30 0.0000E+00 0.0000E+00

```

Figure 7.1 The first lines of the example g2t file created for the surface water exposure assessment for soilless cultivation of substance EXGE1. This file provides the hourly water fluxes and mass fluxes per m² of crop of the substance EXGE1 towards the ditch in the column 'VolOut2SurWat' and 'MasOut2SurWat', respectively.

For the surface water exposure assessment for soil-bound cultivation, files can be found within the folder projects\projectID\assessmentID\PEARL\. A separate file for each substance is created (parent and metabolites). The file has the extension e2t_[substancecnr]. The files provide the water fluxes and substance concentration in these fluxes per m² of cultivated land, while differentiating between runoff overflow, drainage via the micropores and drainage via the bypass (macropores). The data are organized in eight columns as listed below:

1	Time	The simulated time, starting at the start time of the run
2	Date	The simulated date
3	FlvLiqRun	Volume of liquid via runoff overflow per m ² cultivated crop (m ³ d ⁻¹)
4	FlvLiqDraMic	Volume of liquid via micropores and drains per m ² cultivated crop (m ³ d ⁻¹)
5	FlvLiqDraByp	Volume of liquid via macropores and drains per m ² cultivated crop (m ³ d ⁻¹)
6	ConLiqRun	Concentration in the runoff overflow water (kg m ⁻³)
7	ConLiqDraMic	Concentration in the micropore-drain water (kg m ⁻³)
8	ConLiqDraByp	Concentration in the macropore-drain water (kg m ⁻³)


```

-----
* Results from the PEARL model (c) Alterra, PBL and RIVM
* PEARL kernel version : 3.1.5
* SWAP kernel version : swap3237
* PEARL created on : 12-Nov-2014
*
* PEARL was called from : GEM, version 1.1.1
* Working directory : D:\UserData\GEM\Projects\2\3\PEARL
* Run ID : 3
* Input file generated on : 17-12-2014
-----
*
*
* Number of substances: 1
* Parent substance: EXGE1
* NumApp 26
*
* Number Date of application Dosage Soil Cover fraction
* 1 20-Jun-1981 0.6500 1.0000
* 2 20-Jun-1982 0.6500 1.0000
* 3 20-Jun-1983 0.6500 1.0000
* 4 20-Jun-1984 0.6500 1.0000
* 5 20-Jun-1985 0.6500 1.0000
* 6 20-Jun-1986 0.6500 1.0000
* 7 20-Jun-1987 0.6500 1.0000
* 8 20-Jun-1988 0.6500 1.0000
* 9 20-Jun-1989 0.6500 1.0000
* 10 20-Jun-1990 0.6500 1.0000
* 11 20-Jun-1991 0.6500 1.0000
* 12 20-Jun-1992 0.6500 1.0000
* 13 20-Jun-1993 0.6500 1.0000
* 14 20-Jun-1994 0.6500 1.0000
* 15 20-Jun-1995 0.6500 1.0000
* 16 20-Jun-1996 0.6500 1.0000
* 17 20-Jun-1997 0.6500 1.0000
* 18 20-Jun-1998 0.6500 1.0000
* 19 20-Jun-1999 0.6500 1.0000
* 20 20-Jun-2000 0.6500 1.0000
* 21 20-Jun-2001 0.6500 1.0000
* 22 20-Jun-2002 0.6500 1.0000
* 23 20-Jun-2003 0.6500 1.0000
* 24 20-Jun-2004 0.6500 1.0000
* 25 20-Jun-2005 0.6500 1.0000
* 26 20-Jun-2006 0.6500 1.0000
*
* Drain flux and concentration data for substance EXGE1
* Legend to columns:
* Time Date Time FlvLiqRun FlvLiqDraMic FlvLiqDraByp ConLiqRun ConLiqDraMic ConLiqDraByp
* 0.021 01-Jan-1981-00:30 0.0000E+00 0.3900E-04 0.2289E-02 0.0000E+00 0.0000E+00 0.0000E+00
* 0.063 01-Jan-1981-01:30 0.0000E+00 0.3900E-04 0.2289E-02 0.0000E+00 0.0000E+00 0.0000E+00
* 0.104 01-Jan-1981-02:30 0.0000E+00 0.3900E-04 0.2289E-02 0.0000E+00 0.0000E+00 0.0000E+00
* 0.146 01-Jan-1981-03:30 0.0000E+00 0.3900E-04 0.2289E-02 0.0000E+00 0.0000E+00 0.0000E+00
* 0.188 01-Jan-1981-04:30 0.0000E+00 0.3900E-04 0.2289E-02 0.0000E+00 0.0000E+00 0.0000E+00
* 0.229 01-Jan-1981-05:30 0.0000E+00 0.3900E-04 0.2289E-02 0.0000E+00 0.0000E+00 0.0000E+00
* 0.271 01-Jan-1981-06:30 0.0000E+00 0.3900E-04 0.2289E-02 0.0000E+00 0.0000E+00 0.0000E+00
* 0.312 01-Jan-1981-07:30 0.0000E+00 0.3900E-04 0.2289E-02 0.0000E+00 0.0000E+00 0.0000E+00

```

Figure 7.2 The first lines of the example e2t file created for the surface water exposure assessment for soil-bound cultivation of substance EXGE1. This file provides the water fluxes and mass fluxes per hour and per m² of crop of the substance EXGE1 towards the ditch, while differentiating between runoff overflow, drainage via the micropores and drainage via the bypass (macropores).

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Annex 1 DTG crops in GEM

A.1.1 DTG crops for soilless cultivation

In Table A1.1 the soilless grown crops (in greenhouses) of the DTG list are listed. Each of the crops has been assigned to a category with specific water requirements and sodium tolerance. These categories are represented by four crops, being (1) tomato, (2) ficus, (3) rose and (4) sweet pepper (see also Van der Linden *et al.*, 2015). The representative crop, belonging to the assigned category is given in the column 'Reference crop'.

Table A1.1

Soilless grown crops in the GEM instrument.

DTG number				Name of crop	Reference crop
3	2	1		Strawberry	sweet pepper
3	2	4	2	Raspberry	sweet pepper
4	1	1		lettuce	rose
4	1	4	2	Garden cress	rose
4	1	4	3	Watercress	rose
4	2	5	3	Other vegetable sprouts	rose
4	3	1	2	Courgette	tomato
4	3	1	3	Cucumbers	tomato
4	3	3	1	Aubergines	tomato
4	3	3	2	Tomato	tomato
4	3	3	3	Sweet pepper	sweet pepper
5	1	1	1	Basil	ficus
5	1	1	2	Chives	ficus
5	1	1	3	Savoury	ficus
5	1	1	4	Lemon balm	ficus
5	1	1	5	Dill	ficus
5	1	1	6	Tarragon	ficus
5	1	1	9	Coriander	ficus
5	1	1	10	Parsley	ficus
5	1	1	12	Marjoram	ficus
5	1	1	13	Oregano	ficus
5	1	1	14	Mint	ficus
5	1	1	17	Sage	ficus
5	1	1	18	Thyme	ficus
5	3	1	3	Heartsease	ficus
7	1	1	3	Winter Bulb flower and Corm flower forced cultivation	rose
7	1	1	4	Summer Bulb flower and Corm flower forced cultivation	rose
7	2	1	1	Pot plants	ficus
7	2	1	2	Cut flowers	rose
7	2	1	3	Forced shrubs	rose
7	2	1	4	Cut green	rose
7	3	1	4	Climbing plants	ficus
7	3	1	5	Roses	ficus
7	3	1	6	Conifers	ficus
7	3	1	7	Ornamental shrubs	ficus
7	3	1	9	Heather	ficus

A.1.2 DTG crops for soil-bound cultivation

In Table A1.2 the soil-bound greenhouse crops of the DTG list are listed. These can be selected in GEM when a project is started for soil-bound crops cultivation.

Table A1.2

Soil-bound grown crops in the GEM instrument.

DTG number				Name of crop
1	5	1	8	Sugar snaps
4	1	3	1	Spinach
4	1	3	4	Purslane
4	1	4	4	Lamb's lettuce
4	1	4	5	Rocket
4	2	1	1	Bush green beans
4	2	1	5	Climbing common bean
4	2	1	6	Snap bean
4	2	1	7	Runner bean
4	2	3	3	Sugar snap
4	3	1	1	Gherkin
4	4	3	1	Chinese cabbage
4	4	4	1	Kohlrabi
4	5	1	1	Cultivated radish
4	5	1	2	Black/white radish
4	5	2	1	Carrots
4	5	3	6	Beetroot
4	5	3	7	Celeriac
4	7	1	6	Leek
5	1	1	10	Parsley
5	1	1	20	Leaf Celery
7	2	1	2	Cut flowers

Annex 2 Example input file PEARL groundwater

The example input file corresponds to the example project ExProject3.

```

* Input file for PEARL
*
* This file is intended to be used by expert users.
* Figures between brackets refer to constraints (maximum and minimum values).
* Pearl e-mail address: pearl@pesticidemodels.nl
*
* (c) RIVM/PBL/Alterra March 2013
*-----
* Section 0: Run identification and FOCUS 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
*-----
Huissen                Location                Location identification
LightSandyClay         SoilTypeID              Soil identification
STANDARD               CropCalendar            Crop calendar
EXGE2                  SubstanceName           Substance name
ApplicationScheme_GEM  ApplicationScheme       Application scheme
No                     DepositionScheme        Deposition scheme
Waterstromen           IrrigationScheme        Irrigation scheme
*-----
* Section 1: Control section
* Description
*-----
* Release type option CallingProgram
* Options can be: FOCUSPEARL, GEOPEARL, DRAINBOW, EFSAPEARL, BROWSEPEARL, GEM
GEM                    CallingProgram          Release type
1.1.1                  CallingProgramVersion  Version numbers of model, interface and
database
* Time domain
01-Jan-1981            TimStart                Begin time of simulation [01-Jan-1900|-]
31-Dec-2006            TimEnd                  End time of simulation [TimStart|-]
* SWAP control
*No                    RepeatHydrology         Repeat weather data: Yes or No
* 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
Standard              OptHyd                  Option selected to run SWAP

```

```

* If OptHyd is 'Standard' then specify SWAPId to identify SWAP pfo file
Groundwater 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]
9.99           GWLTol        (m)          Tolerance for groundwater level
30             MaxItSwa          Maximum number of iterations in SWAP [1|100]
3             MaxBackTrSwa      Maximum number of bakctrack cycles within an
iteration
0.0001         FacPrecisionPrl (-)       Accuracy criterion in PEARL
* 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 than 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
* For OptAux there are 6 options:
* 1 TOXSWA      : Creates output on drainage and run-off into waterbody to be
simulated by TOXSWA
* 2 TOXSWA-Meta : Creates output using Metamodel TOXSWA
* 3 TOXSWA-All  : Creates output for TOXSWA and Metamodel TOXSWA
* 4 OPS         : Output on emission source strength data for OPS
* 5 All         : Output for both TOXSWA and OPS
* 6 None        : No auxiliary system to be simulated

* If (OptAux == 2 or OptAux == 3) and OptMacropore is 'Yes' then specify OptDitch
* Options for OptDitch are BBW or NMI
NMI          OptDitch          Option for surface water assessment

```



```

*-----
* Section 2: Soil section
* Description
*-----
*If OptSys set to PlantOnly then only Location and SoilTypeID (section 0) are required.
All parameters in section 2 can be omitted if this option has been selected..
* 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)
0.25 25
0.10 8
0.15 3
0.10 2
0.15 3
0.15 2
0.30 3
3.80 38
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 0.826 0.0 0.174 0.121 -99
2 0.855 0.0 0.145 0.010 -99
3 0.855 0.0 0.145 0.010 -99
4 0.855 0.0 0.145 0.010 -99
5 0.855 0.0 0.145 0.010 -99
6 0.855 0.0 0.145 0.010 -99
7 0.855 0.0 0.145 0.010 -99
8 0.855 0.0 0.145 0.010 -99
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

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*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 0.4050 0.050 0.0063 0.0063 1.1712 0.0100 -4.80
*2 0.4050 0.055 0.0278 0.0278 1.1140 0.0287 -9.50
*3 0.3930 0.100 0.0075 0.0075 1.1080 0.0017 -14.45
*4 0.3950 0.010 0.0172 0.0172 1.0925 0.0163 -5.80
*5 0.4440 0.000 0.0117 0.0117 1.0735 0.0251 -0.25
*6 0.4420 0.050 0.0078 0.0078 1.0870 0.0125 -7.70
*7 0.4600 0.010 0.0180 0.0180 1.0500 0.7100 -11.00
*8 0.4600 0.010 0.0180 0.0180 1.0500 0.7100 -11.00
*end_table
* If OptMacropore 'Yes' then extended table VanGenuchtenPar
table horizon VanGenuchtenPar
Nr ThetaSat ThetaRes AlphaDry AlphaWet n KSat l PreHeaEnt
CofAniso
(m3.m-3) (m3.m-3) (cm-1) (cm-1) (-) (m.d-1) (-) (cm) (-)
1 0.53 0.01 0.0242 0.0242 1.280 0.8128 -1.476 0.0 1.0
2 0.46 0.0 0.0194 0.0094 1.4 0.0223 -1.332 0.0 1.0
3 0.46 0.0 0.0194 0.0094 1.4 0.0223 -1.332 0.0 1.0
4 0.46 0.0 0.0194 0.0094 1.4 0.0223 -1.332 0.0 1.0
5 0.46 0.0 0.0194 0.0094 1.4 0.0223 -1.332 0.0 1.0
6 0.46 0.0 0.0194 0.0094 1.4 0.0223 -1.332 0.0 1.0
7 0.46 0.0 0.0194 0.0094 1.4 0.0223 -1.332 0.0 1.0
8 0.46 0.0 0.0194 0.0094 1.4 0.0223 -1.332 0.0 1.0
end_table
Calculate 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]
end_table
* End If
* 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
1.0 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]
0.6667 ExpDifLiqMilDen (-) Exponent in denominator of eqn [0.1|2]
2.0 ExpDifGasMilNom (-) Exponent in nominator of equation [0.1|5]
0.6667 ExpDifGasMilDen (-) Exponent in denominator of eqn [0.1|2]

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* 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  0.1
7  0.1
8  0.1
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)
Yes          OptMacroporePTF    Simulate macropore flow (Yes|No)
0.000       ZPndMacMax      (m)      Maximum ponding depth for runoff into the
              macropores
-0.25       ZAHor          (m)      Depth of A-horizon
0.0         FraZAHor      (-)      Fraction of macropores ended at Z=ZAh
*-0.80      ZIca          (m)      Bottom of internal catchment domain
*-1.60      ZSta          (m)      Bottom of static macropores
-2.48392   GLG           (m)      Bottom of static macropores
1.0         PowMac        (-)      Power in distribution internal catchment domain
*0.03       VolStaTop     (m3.m-3) Volume of static macropores at soil surface
*0.90       FraIcaTop     (-)      Fraction of internal catchment domain at soil
              surface
*0.031     DiaPolMin     (m)      Minimum diameter of soil polygons (soil surface)
*0.155     DiaPolMax     (m)      Maximum diameter of soil polygons (deep)
14.0       RstDraRapRef  (d-1)    Reference rapid drainage resistance
1.0        RstDraRapExp  (-)      Rapid drainage exponent
0.125     FraThiLayMix  (-)      Runoff extraction efficiency factor
0.02      FraSorByp     (-)      Fraction of sorption sites in bypass domain
* If (OptAux == 2 or OptAux == 3) and OptMacropore is 'Yes' then specify Ditch
properties
* hydrotypes 18 (Westland-DC profiel)
100.0     AreaField     (m2.m-1)
200.0     AreaUpstream  (m2.m-1)
1.0       FraUpstreamTreated  (-)
2.0       ParAlphaTOXSWA  (-)

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1.1383      VolDitch1      (m3.m-1)
2.84       WidthDitch1     (m)
0.01      LenDitch1      (m.m-2)
* End if
*-----
* Section 3: Weather and irrigation data
* Description
*-----
Rotterdam      MeteoStation      Maximum 7 characters.
Input          OptEvp            Evapotranspiration: Input, Penman,
               PenmanMonteith or Makkink
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
20.0          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
Waterstromen      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
100.0        LenFld (m)
2.0          ZMeaTem (m)
Yes          OptRainfallEvents      Specify event based rainfall events
0.04        LenRainfall (d)      Duration of rainfall events
No          OptSnow          Option to consider snow in SWAP
*-----
* Section 4: Boundary and initial conditions of hydrological model
* Section 4a: Lower boundary flux conditions
* Description
*-----

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*-----
* Initial condition
-150.0          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
      Cauchy          OptLbo          Lower boundary option selected
* If OptLbo = 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 OptLbo = 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 OptLbo = Cauchy then specify lower boundary option
* Options for bottom flux can be Sine, HeadOnly or HeadAndFlux
HeadAndFlux        OptBotFlux          Option selected for bottom flux
No                  OptNoResVert        Switch on or switch off vertical resistance
NoDrains           OptShapeGrwLev       Elliptic, Parabolic, Sinusoidal, NoDrains
-1.06              HeaDraBase          (m)          Drainage base to correct GrwLev [-100|0]
158.00             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
11_5887_gw 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 OptLbo = 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]

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* OptLbo = 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
*-----
Basic          OptDra          No, Basic or extended drainage module
1              NumDraLev      Number of drainage levels (0|5)
* If OptDra =\ No then NumDraLev cannot be zero.
* If OptDra =\ 0 then specify switch to adjust upper boundary of model discharge layer
No             OptDisLay      Option selected for discharge layer
* If OptDra set to 'Basic' parameters below should be specified for each drainage level:
1              SysDra_1       Drainage system
986.0         RstDra_1        (d)      Drainage resistance [10|1e5]
10000         RstInf_1        (d)      Infiltration resistance
359.0         DistDra_1       (m)      Distance between drains or channels [1|1e6]
1.06          ZDra_1         (m)      Bottom of drain system [0|10]
Channel       TypDra_1       Type of drain system: Drain or Channel
*0.76         ZSurWat_1       (m)      Channel water level (if TypDra_1 = Channel;
otherwise dummy values)
0.76          ZSurWatSum_1    (m)      Channel water level (if TypDra_1 = Channel;
otherwise dummy values)
0.76          ZSurWatWin_1    (m)      Channel water level (if TypDra_1 = Channel;
otherwise dummy values)
No             OptSurDra      Option to consider rapid subsurface drainage
* If OptSurDra set to 'Yes' then the following parameters should be specified:
* 30          RstSurDraDeep   (d)      maximum resistance of rapid subsurface *drainage
[1e-3|1e4]]
* 10          RstSurDraShallow(d)      minimum resistance of rapid subsurface drainage
[1e-3|1e4]]
* No          OptSrfWat       Option to consider surface water system
* If OptSrfWat set to 'Yes' then the following parameters should be specified:
* 1.0         SrfWatLevWinter (m)      Winter surface water level
* 1.0         SrfWatLevSummer (m)      Summer surface water level
* 0.0         SrfWatSupCap    (m.d-1)  Surface water supply capacity
*-----
* Section 5: Compound section
* Description
*-----
* Compounds. First compound is the parent pesticide, the others are metabolites.
EXGE2
EXGE3
end_table
200.          MolMas_EXGE2 (g.mol-1)    Molar mass [10|10000]
150.          MolMas_EXGE3 (g.mol-1)    Molar mass [10|10000]
* Transformation table (parent-daughter relationships)
* The "end" substance is the final transformation product
* Condition: Sum of rows should be 1 (see theory document)
table FraPrtDau (mol.mol-1)
0.71 EXGE2 -> EXGE3
end_table

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* Example for a pesticide with two daughters, named "met1" and "met2":
* Line 1: pest is transformed into met1 (25%), met2 (70%) and undefined end products (5%)
* Line 2: met1 is transformed into met2 (16%) and undefined end products (84%)
* Line 3: met2 is transformed into undefined end products only (100%)
* table FraPrtDau (mol.mol-1)
* pest    met1    met2    end
* 0.00    0.25    0.70    0.05    pest
* 0.00    0.00    0.16    0.84    met1
* 0.00    0.00    0.00    1.00    met2
* end_table
* Transformation rate parameters
EqlDom_Input          OptDT50_EXGE2          Option for DT50: Input or Calculate in
                        equilibrium domain (EqlDom) or in liquid phase
                        only (LiqPhs)
20.                    DT50Ref_EXGE2 (d)      Half-life time [1|1e6]
20.                    TemRefTra_EXGE2 (C)    Temperature at which DT50 is measured [5|30]
0.7                    ExpLiqTra_EXGE2 (-)    Exponent for the effect of liquid [0|5]
NonOptimumConditions OptCntLiqTraRef_EXGE2    OptimumConditions or NonOptimumConditions
1.                    CntLiqTraRef_EXGE2 (kg.kg-1)  Liq. content at which DT50 is measured [0|1]
65.4                  MolEntTra_EXGE2 (kJ.mol-1)  Molar activation energy [0|200]
EqlDom_Input          OptDT50_EXGE3          Option for DT50: Input or Calculate in
                        equilibrium domain (EqlDom) or in liquid phase
                        only (LiqPhs)
100.                  DT50Ref_EXGE3 (d)      Half-life time [1|1e6]
20.                    TemRefTra_EXGE3 (C)    Temperature at which DT50 is measured [5|30]
0.7                    ExpLiqTra_EXGE3 (-)    Exponent for the effect of liquid [0|5]
NonOptimumConditions OptCntLiqTraRef_EXGE3    OptimumConditions or NonOptimumConditions
1.                    CntLiqTraRef_EXGE3 (kg.kg-1)  Liq. content at which DT50 is measured [0|1]
65.4                  MolEntTra_EXGE3 (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 interpolate FacZTra (-)
hor EXGE2 EXGE3
0.00 1.00 1.00
0.30 1.00 1.00
0.31 0.50 0.50
0.60 0.50 0.50
0.61 0.30 0.30
1.00 0.30 0.30
1.01 0.00 0.00
5.00 0.00 0.00
end_table
* Freundlich equilibrium sorption
pH-independent OptCofFre_EXGE2          pH-dependent, pH-independent, CofFre
1.            ConLiqRef_EXGE2 (mg.L-1)  Reference conc. in liquid phase [0.1|-]
0.9          ExpFre_EXGE2 (-)           Freundlich sorption exponent [0.1|1.3]
pH-independent OptCofFre_EXGE3          pH-dependent, pH-independent, CofFre
1.            ConLiqRef_EXGE3 (mg.L-1)  Reference conc. in liquid phase [0.1|-]
0.9          ExpFre_EXGE3 (-)           Freundlich sorption exponent [0.1|1.3]
* If pH-independent (use the coefficient for sorption on organic matter):
100.         KomEq1_EXGE2 (L.kg-1)      Coef. eql. sorption on org. matter [0|1e9]
100.         KomEq1Max_EXGE2 (L.kg-1)   Coef. eql. sorption on org. matter in dry soil
[0|1e9]
30.          KomEq1_EXGE3 (L.kg-1)      Coef. eql. sorption on org. matter [0|1e9]
30.          KomEq1Max_EXGE3 (L.kg-1)   Coef. eql. sorption on org. matter in dry soil
[0|1e9]

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* If pH-dependent (use pKa value and coefficient for sorption on organic matter):
    KomEqAcid_EXGE2 (L.kg-1)   Coef. for eql. sorption on om - acid [0|1e9]
    KomEqBase_EXGE2 (L.kg-1)   Coef. for eql. sorption on om - base [0|1e9]
    pKa_EXGE2         (-)       Coef. for influence of pH on sorption [0|14]
    pHCorrection      (-)       pH correction [-2|1]

    KomEqAcid_EXGE3 (L.kg-1)   Coef. for eql. sorption on om - acid [0|1e9]
    KomEqBase_EXGE3 (L.kg-1)   Coef. for eql. sorption on om - base [0|1e9]
    pKa_EXGE3         (-)       Coef. for influence of pH on sorption [0|14]

* If CofFre (specify the depth dependence and the coefficient for equilibrium sorption):
    KSorEqL_EXGE2 (L.kg-1)   Coef. for equilibrium sorption [0|1e9]
0.    MolEntSor_EXGE2 (kJ.mol-1)
20.   TemRefSor_EXGE2 (C)

    KSorEqL_EXGE3 (L.kg-1)   Coef. for equilibrium sorption [0|1e9]
0.    MolEntSor_EXGE3 (kJ.mol-1)
20.   TemRefSor_EXGE3 (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 interpolate FacZSor (-)          Factor for the effect of depth [0|1]
hor EXGE2 EXGE3
1 -99 -99
2 -99 -99
3 -99 -99
4 -99 -99
5 -99 -99
6 -99 -99
7 -99 -99
8 -99 -99
end_table
* End If
* Gas/liquid partitioning
1.E-10    PreVapRef_EXGE2 (Pa)          Saturated vapour pressure [0|2e5]
20.       TemRefVap_EXGE2 (C)          .. measured at [0|40]
95.       MolEntVap_EXGE2 (kJ.mol-1)   Molar enthalpy of vaporisation [-200|200]
50.       SlbWatRef_EXGE2 (mg.L-1)     Solubility in water [1e-9|1e6]
20.       TemRefSlb_EXGE2 (C)          .. measured at [0|40]
27.       MolEntSlb_EXGE2 (kJ.mol-1)   Molar enthalpy of dissolution [-200|200]

1.E-10    PreVapRef_EXGE3 (Pa)          Saturated vapour pressure [0|2e5]
20.       TemRefVap_EXGE3 (C)          .. measured at [0|40]
95.       MolEntVap_EXGE3 (kJ.mol-1)   Molar enthalpy of vaporisation [-200|200]
90.       SlbWatRef_EXGE3 (mg.L-1)     Solubility in water [1e-9|1e6]
20.       TemRefSlb_EXGE3 (C)          .. measured at [0|40]
27.       MolEntSlb_EXGE3 (kJ.mol-1)   Molar enthalpy of dissolution [-200|200]

* Non-equilibrium sorption
0.        CofDesRat_EXGE2 (d-1)        Desorption rate coefficient [0|0.5]
0.        FacSorNeqEqL_EXGE2 (-)       CofFreNeq/CofFreEqL [0|-]

0.        CofDesRat_EXGE3 (d-1)        Desorption rate coefficient [0|0.5]
0.        FacSorNeqEqL_EXGE3 (-)       CofFreNeq/CofFreEqL [0|-]

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* Uptake
0.5          FacUpt_EXGE2 (-)          Coefficient for uptake by plant [0|10]
0.5          FacUpt_EXGE3 (-)          Coefficient for uptake by plant [0|10]
* Canopy processes
Lumped      OptDspCrp_EXGE2 (d)        Lumped, Specified or Calculated
Lumped      OptDspCrp_EXGE3 (d)        Lumped, Specified or Calculated
* If Lumped:
1000000.    DT50DspCrp_EXGE2 (d)        Half-life at crop surface [1|1e6]
1000000.    DT50DspCrp_EXGE3 (d)        Half-life at crop surface [1|1e6]
* If Specified:
            DT50PenCrp_EXGE2 (d)        Half-life due to penetration [1|1e6]
            DT50VolCrp_EXGE2 (d)        Half-life due to volatilization [1|1e6]
            DT50TraCrp_EXGE2 (d)        Half-life due to transformation [1|1e6]
            DT50PenCrp_EXGE3 (d)        Half-life due to penetration [1|1e6]
            DT50VolCrp_EXGE3 (d)        Half-life due to volatilization [1|1e6]
            DT50TraCrp_EXGE3 (d)        Half-life due to transformation [1|1e6]
* If Calculated:
            DT50PenCrp_EXGE2 (d)        Half-life due to penetration [1|1e6]
            DT50TraCrp_EXGE2 (d)        Half-life due to photo-transformation [1|1e6]
            DT50PenCrp_EXGE3 (d)        Half-life due to penetration [1|1e6]
            DT50TraCrp_EXGE3 (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
0.0001      FacWasCrp_EXGE2 (m-1)        Wash-off factor [1e-6|0.1]
0.0001      FacWasCrp_EXGE3 (m-1)        Wash-off factor [1e-6|0.1]
* Diffusion of solute in liquid and gas phases
4.3E-5      CofDifWatRef_EXGE2 (m2.d-1) Reference diff. coeff. in water [10e-5|3e-4]
0.43       CofDifAirRef_EXGE2 (m2.d-1) Reference diff. coeff. in air [0.1|3]
20.        TemRefDif_EXGE2 (C)          Diff. coeff measured at temperature [10|30]

4.3E-5      CofDifWatRef_EXGE3 (m2.d-1) Reference diff. coeff. in water [10e-5|3e-4]
0.43       CofDifAirRef_EXGE3 (m2.d-1) Reference diff. coeff. in air [0.1|3]
20.        TemRefDif_EXGE3 (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]
0.3        ZTil                (m)

```

```

* Event table:
* Column 1: Date* Column 2: Event type: AppSolSur, AppSolInj, AppSolTil, AppCrpUsr,
AppCrpLAI
* AppSolSur, AppSolInj, AppSolTil cannot be combined with OptSys set to PlantOnly
* 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]
* End If
table Applications
08-Apr      AppSolSur      0.7000
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
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 CntSysEq1              (mg.kg-1)
0.0000  0.000
50.000  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
50.000  0.000
end_table
* Upper boundary flux                      [0|-]
table FlmDep (kg.ha-1.d-1)
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
01-Jan      31-Dec      STANDARD
end_table

```

```

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

* If OptLenCrp = Variable:
*0.0          TemSumSta_STANDARD (C)           Start value of temperature sum [-10|20]
*0.0          TemSumEmgAnt_STANDARD (C)        Sum from emergence to anthesis [0|1e4]
*0.0          TemSumAntMat_STANDARD (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_STANDARD
0.000  12  1.0  0.30  0.60
1.000  12  1.0  0.30  0.60
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_STANDARD
0.000  1.0
1.0    1.0
end_table

* Crop water use
100.0          HLim1_STANDARD (cm)           Anaerobiosis point [-100|0]
100.0          HLim2_STANDARD (cm)           Wet reduction point [-1000|0]
-1000.0        HLim3U_STANDARD (cm)          Dry reduction point [-10000|0]
-1000.0        HLim3L_STANDARD (cm)          Dry reduction point [-10000|0]
-16000.0       HLim4_STANDARD (cm)           Wilting point [-16000|0]

70.0           RstEvpCrp_STANDARD (s.m-1)     Min. canopy resistance [0|1000]
0.39           CofExtDif_STANDARD (-)
1.0            CofExtDir_STANDARD (-)
*0.2           ZTensioMeter_STANDARD (m)
-1000.0        PreHeaIrrSta_STANDARD (cm)
0.0            CofIntCrp_STANDARD (cm)        Constant in Braden eq for interception [0|1]
*15.0          IrgThreshold_STANDARD (mm)     Threshold of moisture deficit to allow
                                                    irrigation

0.0            RstEvpIntCrp_STANDARD

-----
* Section 9: Output control
* Description
*-----
LAST SECTION-NOT SHOWN HERE

```

Annex 3 Example input file PEARL surface water

The example input file corresponds to the example project ExProject2

```

* Input file for PEARL
*
* This file is intended to be used by expert users.
* Figures between brackets refer to constraints (maximum and minimum values).
* Pearl e-mail address: pearl@pesticidemodels.nl
*
* (c) RIVM/PBL/Alterra March 2013
*-----
* Section 0: Run identification and FOCUS 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
*-----
Bleiswijk           Location           Location identification
SandyClay           SoilTypeID        Soil identification *upper soillayer is
B15; structure comes from WUR horticulture
STANDARD            CropCalendar      Crop calendar
EXGEL               SubstanceName     Substance name
ApplicationScheme_GEM ApplicationScheme  Application scheme
No                  DepositionScheme  Deposition scheme
Waterstromen        IrrigationScheme  Irrigation scheme
*-----
* Section 1: Control section
* Description
*-----
* Release type option CallingProgram
* Options can be: FOCUSPEARL, GEOPEARL, DRAINBOW, EFSAPEARL, BROWSEPEARL, GEM
GEM                 CallingProgram    Release type
1.1.1               CallingProgramVersion Version numbers of model, interface and
database
* Time domain
01-Jan-1981         TimStart          Begin time of simulation [01-Jan-1900|-]
31-Dec-2006         TimEnd            End time of simulation [TimStart|-]
* SWAP control
*No                 RepeatHydrology   Repeat weather data: Yes or No
* 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

```

```

* If OptHyd is 'Standard' then specify SWAPID to identify SWAP pfo file
Surfacewater SwapID          Dutch surface water standard scenario for
summer
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]
9.99          GWLTol       (m)       Tolerance for groundwater level
30            MaxItSwa      Maximum number of iterations in SWAP [1|100]
3            MaxBackTrSwa   Maximum number of bakctrack cycles within an
iteration
0.0001        FacPrecisionPrl (-)    Accuracy criterion in PEARL
* 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 than 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
TOXSWA      OptAux             Option for auxiliary output
* For OptAux there are 6 options:
* 1 TOXSWA      : Creates output on drainage and run-off into waterbody to be
simulated by TOXSWA
* 2 TOXSWA-Meta : Creates output using Metamodel TOXSWA
* 3 TOXSWA-All  : Creates output for TOXSWA and Metamodel TOXSWA
* 4 OPS        : Output on emission source strength data for OPS
* 5 All        : Output for both TOXSWA and OPS
* 6 None       : No auxiliary system to be simulated

* If (OptAux == 2 or OptAux == 3) and OptMacropore is 'Yes' then specify OptDitch
* Options for OptDitch are BBW or NMI
NMI          OptDitch           Option for surface water assessment

```

```

*-----
* Section 2: Soil section
* Description
*-----
*If OptSys set to PlantOnly then only Location and SoilTypeID (section 0) are required.
All parameters in section 2 can be omitted if this option has been selected..
* 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)
0.25 25
0.10 8
0.15 3
0.10 2
0.15 3
0.15 2
0.30 3
3.80 38
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 0.775 0.0 0.225 0.137 -99
2 0.365 0.0 0.635 0.015 -99
3 0.365 0.0 0.635 0.015 -99
4 0.365 0.0 0.635 0.015 -99
5 0.365 0.0 0.635 0.015 -99
6 0.365 0.0 0.635 0.015 -99
7 0.365 0.0 0.635 0.015 -99
8 0.365 0.0 0.635 0.015 -99
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 0.4050 0.050 0.0063 0.0063 1.1712 0.0100 -4.80
*2 0.4050 0.055 0.0278 0.0278 1.1140 0.0287 -9.50
*3 0.3930 0.100 0.0075 0.0075 1.1080 0.0017 -14.45
*4 0.3950 0.010 0.0172 0.0172 1.0925 0.0163 -5.80
*5 0.4440 0.000 0.0117 0.0117 1.0735 0.0251 -0.25
*6 0.4420 0.050 0.0078 0.0078 1.0870 0.0125 -7.70
*7 0.4600 0.010 0.0180 0.0180 1.0500 0.7100 -11.00
*8 0.4600 0.010 0.0180 0.0180 1.0500 0.7100 -11.00
*end_table
* If OptMacropore 'Yes' then extended table VanGenuchtenPar
table horizon VanGenuchtenPar
Nr ThetaSat ThetaRes AlphaDry AlphaWet n KSat l PreHeaEnt
CofAniso
(m3.m-3) (m3.m-3) (cm-1) (cm-1) (-) (m.d-1) (-) (cm) (-)
1 0.53 0.01 0.0242 0.0242 1.280 0.8128 -1.476 0.0 1.0
2 0.57 0.0 0.0194 0.0194 1.089 0.0437 -5.955 0.0 1.0
3 0.57 0.0 0.0194 0.0194 1.089 0.0437 -5.955 0.0 1.0
4 0.57 0.0 0.0194 0.0194 1.089 0.0437 -5.955 0.0 1.0
5 0.57 0.0 0.0194 0.0194 1.089 0.0437 -5.955 0.0 1.0
6 0.57 0.0 0.0194 0.0194 1.089 0.0437 -5.955 0.0 1.0
7 0.57 0.0 0.0194 0.0194 1.089 0.0437 -5.955 0.0 1.0
8 0.57 0.0 0.0194 0.0194 1.089 0.0437 -5.955 0.0 1.0
end_table
Calculate 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]
end_table
* End If
* 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
1.0 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]
0.6667 ExpDifLiqMilDen (-) Exponent in denominator of eqn [0.1|2]
2.0 ExpDifGasMilNom (-) Exponent in nominator of equation [0.1|5]
0.6667 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  0.1
7  0.1
8  0.1
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'
-----
Yes          OptMacropore      Simulate macropore flow (Yes|No)
Yes          OptMacroporePTF    Simulate macropore flow (Yes|No)
0.000       ZPndMacMax      (m)      Maximum ponding depth for runoff into the
              macropores
-0.25       ZAHor          (m)      Depth of A-horizon
0.0         FraZAHor      (-)      Fraction of macropores ended at Z=ZAh
*-0.80      ZIca          (m)      Bottom of internal catchment domain
*-1.60      ZSta          (m)      Bottom of static macropores
-1.39185   GLG           (m)      Bottom of static macropores
1.0         PowMac        (-)      Power in distribution internal catchment domain
*0.03       VolStaTop     (m3.m-3) Volume of static macropores at soil surface
*0.90       FraIcaTop     (-)      Fraction of internal catchment domain at soil
              surface
*0.031     DiaPolMin     (m)      Minimum diameter of soil polygons (soil surface)
*0.155     DiaPolMax     (m)      Maximum diameter of soil polygons (deep)
10.0       RstDraRapRef  (d-1)    Reference rapid drainage resistance
1.0        RstDraRapExp  (-)      Rapid drainage exponent
0.125     FraThiLayMix (-)      Runoff extraction efficiency factor
0.02      FraSorByp     (-)      Fraction of sorption sites in bypass domain
* If (OptAux == 2 or OptAux == 3) and OptMacropore is 'Yes' then specify Ditch
properties
* hydrottype 18 (Westland-DC profiel)
100.0     AreaField     (m2.m-1)
200.0     AreaUpstream (m2.m-1)
1.0       FraUpstreamTreated (-)
2.0       ParAlphaTOXSWA (-)

```

```

0.5699      VolDitch1      (m3.m-1)
2.50        WidthDitch1      (m)
0.01        LenDitch1      (m.m-2)
* End if
*-----
* Section 3: Weather and irrigation data
* Description
*-----
Rotterdam      MeteoStation      Maximum 7 characters.
Input          OptEvp            Evapotranspiration: Input, Penman,
                PenmanMonteith or Makkink
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
20.0          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
Waterstromen      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
100.0          LenFld (m)
2.0            ZMeaTem (m)
Yes            OptRainfallEvents      Specify event based rainfall events
0.04          LenRainfall      (d)      Duration of rainfall events
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
-80.0          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
      Cauchy          OptLbo          Lower boundary option selected
* If OptLbo = 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 OptLbo = 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 OptLbo = Cauchy then specify lower boundary option
* Options for bottom flux can be Sine, HeadOnly or HeadAndFlux
HeadAndFlux        OptBotFlux          Option selected for bottom flux
Yes                OptNoResVert        Switch on or switch off vertical resistance
NoDrains           OptShapeGrwLev      Elliptic, Parabolic, Sinusoidal, NoDrains
-0.90              HeaDraBase          (m)          Drainage base to correct GrwLev [-100|0]
320.00             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
05_6211_sw 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 OptLbo = 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]

```

```

* OptLbo = 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
*-----
Basic          OptDra          No, Basic or extended drainage module
1              NumDraLev       Number of drainage levels (0|5)
* If OptDra =\ No then NumDraLev cannot be zero.
* If OptDra =\ 0 then specify switch to adjust upper boundary of model discharge layer
No            OptDisLay       Option selected for discharge layer
* If OptDra set to 'Basic' parameters below should be specified for each drainage level:
1            SysDra_1         Drainage system
971.0        RstDra_1         (d)      Drainage resistance [10|1e5]
10000        RstInf_1         (d)      Infiltration resistance
3.2          DistDra_1        (m)      Distance between drains or channels [1|1e6]
0.9          ZDra_1           (m)      Bottom of drain system [0|10]
Drain        TypDra_1         Type of drain system: Drain or Channel
0.90         ZSurWat_1        (m)      Channel water level (if TypDra_1 = Channel;
                                   otherwise dummy values)
* If OptDra set to 'Extended' parameters below should be specified for each drainage level:
* 1          SysDra_1         Drainage system
* 100.0      RstDra_1         (d)      Drainage resistance [10|1e5]
* 100.0      RstInf_1         (d)      Infiltration resistance
* 20.0       DistDra_1        (m)      Distance between drains or channels [1|1e6]
* 1.0        WidthDra_1       (m)      Bottom width of drain system
* 1.5        ZDra_1           (m)      Bottom of drain system [0|10]
* 1.5        ZGwlInfMax_1     (m)      Depth at which infiltration is maximal
No           OptSurDra       Option to consider rapid subsurface drainage
* If OptSurDra set to 'Yes' then the following parameters should be specified:
* 30         RstSurDraDeep    (d)      maximum resistance of rapid subsurface *drainage
                                   [1e-3|1e4]]
* 10         RstSurDraShallow(d) minimum resistance of rapid subsurface drainage
                                   [1e-3|1e4]]
* No         OptSrfWat       Option to consider surface water system
* If OptSrfWat set to 'Yes' then the following parameters should be specified:
* 1.0        SrfWatLevWinter (m)      Winter surface water level
* 1.0        SrfWatLevSummer (m)      Summer surface water level
* 0.0        SrfWatSupCap    (m.d-1)  Surface water supply capacity
*-----
* Section 5: Compound section
* Description
*-----
* Compounds. First compound is the parent pesticide, the others are metabolites.
table compounds
EXGE1
end_table
255.7        MolMas_EXGE1 (g.mol-1)    Molar mass [10|10000]
* Transformation table (parent-daughter relationships)
* The "end" substance is the final transformation product
* Condition: Sum of rows should be 1 (see theory document)
table FraPrtDau (mol.mol-1)
end_table

```

```

* Example for a pesticide with two daughters, named "met1" and "met2":
* Line 1: pest is transformed into met1 (25%), met2 (70%) and undefined end products (5%)
* Line 2: met1 is transformed into met2 (16%) and undefined end products (84%)
* Line 3: met2 is transformed into undefined end products only (100%)
* table FraPrtDau (mol.mol-1)
* pest    met1    met2    end
* 0.00    0.25    0.70    0.05    pest
* 0.00    0.00    0.16    0.84    met1
* 0.00    0.00    0.00    1.00    met2
* end_table
* Transformation rate parameters
EqLDom_Input          OptDT50_EXGE1          Option for DT50: Input or Calculate in
                        equilibrium domain (EqLDom) or in liquid phase
                        only (LiqPhs)
117.7                  DT50Ref_EXGE1    (d)          Half-life time [1|1e6]
20.                    TemRefTra_EXGE1 (C)          Temperature at which DT50 is measured [5|30]
0.7                    ExpLiqTra_EXGE1 (-)          Exponent for the effect of liquid [0|5]
OptimumConditions     OptCntLiqTraRef_EXGE1          OptimumConditions or NonOptimumConditions
                        CntLiqTraRef_EXGE1 (kg.kg-1)  Liq. content at which DT50 is measured [0|1]
65.4                   MolEntTra_EXGE1    (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 interpolate FacZTra (-)
hor EXGE1
0.00 1.00
0.30 1.00
0.31 0.50
0.60 0.50
0.61 0.30
1.00 0.30
1.01 0.00
5.00 0.00
end_table

* Freundlich equilibrium sorption
pH-independent         OptCofFre_EXGE1          pH-dependent, pH-independent, CofFre
1.                     ConLiqRef_EXGE1 (mg.L-1)  Reference conc. in liquid phase [0.1|-]
0.9                    ExpFre_EXGE1 (-)        Freundlich sorption exponent [0.1|1.3]
* If pH-independent (use the coefficient for sorption on organic matter):
131.                   KomEqL_EXGE1    (L.kg-1)    Coef. eql. sorption on org. matter [0|1e9]
131.                   KomEqLMax_EXGE1 (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):
                        KomEqLAcid_EXGE1 (L.kg-1)    Coef. for eql. sorption on om - acid [0|1e9]
                        KomEqLBase_EXGE1 (L.kg-1)    Coef. for eql. sorption on om - base [0|1e9]
                        pKa_EXGE1          (-)        Coef. for influence of pH on sorption [0|14]
                        pHCorrection      (-)        pH correction [-2|1]
* If CofFre (specify the depth dependence and the coefficient for equilibrium sorption):
                        KSorEqL_EXGE1    (L.kg-1)    Coef. for equilibrium sorption [0|1e9]
0.                     MolEntSor_EXGE1    (kJ.mol-1)
20.                    TemRefSor_EXGE1    (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 interpolate FacZSor (-)          Factor for the effect of depth [0|1]

```

```

hor EXGE1
1 -99
2 -99
3 -99
4 -99
5 -99
6 -99
7 -99
8 -99
end_table
* End If
* Gas/liquid partitioning
4.E-10      PreVapRef_EXGE1 (Pa)      Saturated vapour pressure [0|2e5]
20.         TemRefVap_EXGE1 (C)      .. measured at [0|40]
95.         MolEntVap_EXGE1 (kJ.mol-1) Molar enthalpy of vaporisation [-200|200]
613.       SlbWatRef_EXGE1 (mg.L-1) Solubility in water [1e-9|1e6]
20.         TemRefSlb_EXGE1 (C)     .. measured at [0|40]
27.         MolEntSlb_EXGE1 (kJ.mol-1) Molar enthalpy of dissolution [-200|200]

* Non-equilibrium sorption
0.          CofDesRat_EXGE1 (d-1)    Desorption rate coefficient [0|0.5]
0.          FacSorNeqEqL_EXGE1 (-)   CofFreNeq/CofFreEqL [0|-]
* Uptake
0.5         FacUpt_EXGE1 (-)         Coefficient for uptake by plant [0|10]
* Canopy processes
Lumped      OptDspCrp_EXGE1 (d)      Lumped, Specified or Calculated
* If Lumped:
10.         DT50DspCrp_EXGE1 (d)     Half-life at crop surface [1|1e6]
* If Specified:
           DT50PenCrp_EXGE1 (d)     Half-life due to penetration [1|1e6]
           DT50VolCrp_EXGE1 (d)     Half-life due to volatilization [1|1e6]
           DT50TraCrp_EXGE1 (d)     Half-life due to transformation [1|1e6]
* If Calculated:
           DT50PenCrp_EXGE1 (d)     Half-life due to penetration [1|1e6]
           DT50TraCrp_EXGE1 (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
0.0001     FacWasCrp_EXGE1 (m-1)     Wash-off factor [1e-6|0.1]
* Diffusion of solute in liquid and gas phases
4.3E-5     CofDifWatRef_EXGE1 (m2.d-1) Reference diff. coeff. in water [10e-5|3e-4]
0.43      CofDifAirRef_EXGE1 (m2.d-1) Reference diff. coeff. in air [0.1|3]
20.       TemRefDif_EXGE1 (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]
0.3        ZTil           (m)

```

```

* Event table:
* Column 1: Date* Column 2: Event type: AppSolSur, AppSolInj, AppSolTil, AppCrpUsr,
AppCrpLAI
* AppSolSur, AppSolInj, AppSolTil cannot be combined with OptSys set to PlantOnly
* 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]
* End If
table Applications
20-Jun      AppSolSur      0.6500
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
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 CntSysEq1              (mg.kg-1)
0.0000  0.000
50.000  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
50.000  0.000
end_table
* Upper boundary flux                      [0|-]
table FlmDep (kg.ha-1.d-1)
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
01-Jan      31-Dec      STANDARD
end_table
table IrrigationPeriods
01-Jan      31-Dec      STANDARD
end_table

```

```

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

* If OptLenCrp = Variable:
*0.0          TemSumSta_STANDARD      (C)          Start value of temperature sum [-10|20]
*0.0          TemSumEmgAnt_STANDARD   (C)          Sum from emergence to anthesis [0|1e4]
*0.0          TemSumAntMat_STANDARD   (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_STANDARD
0.000  12  1.0  0.30  0.60
1.000  12  1.0  0.30  0.60
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_STANDARD
0.000  1.0
1.0    1.0
end_table

* Crop water use
100.0          HLim1_STANDARD (cm)          Anaerobiosis point [-100|0]
100.0          HLim2_STANDARD (cm)          Wet reduction point [-1000|0]
-1000.0        HLim3U_STANDARD (cm)          Dry reduction point [-10000|0]
-1000.0        HLim3L_STANDARD (cm)          Dry reduction point [-10000|0]
-16000.0       HLim4_STANDARD (cm)          Wilting point [-16000|0]

70.0          RstEvpCrp_STANDARD (s.m-1)      Min. canopy resistance [0|1000]
0.39          CofExtDif_STANDARD (-)
1.0          CofExtDir_STANDARD (-)
*0.2          ZTensioMeter_STANDARD (m)
-1000.0       PreHeaIrrSta_STANDARD (cm)
0.0          CofIntCrp_STANDARD (cm)          Constant in Braden eq for interception [0|1]
*15.0         IrgThreshold_STANDARD (mm)      Threshold of moisture deficit to allow
                                                    irrigation

0.0          RstEvpIntCrp_STANDARD

-----
* Section 9: Output control
* Description
*-----
LAST SECTION-NOT SHOWN HERE

```

Annex 4 Example input file TOXSWA

The example input file corresponds to the example project ExProject2

```

* INPUT FILE for TOXSWA
*-----
* * Contact address:
* Wim Beltman
* Alterra
* PO BOX 47
* 6700 AA Wageningen
* The Netherlands
* e-mail: wim.beltman@wur.nl
* * (c) Alterra
*-----
* Section 1: Control section
*-----
01-Jan-2000      TimStart   ! Starting time of simulation [01-Jan-1900 - 31-Dec-9999]
31-Dec-2006      TimEnd     ! End time of simulation [01-Jan-1900 - 31-Dec-9999]
* Version of calling program (CallingProgram):
* NL             = in DRAINBOW for Dutch authorization
GEM             CallingProgram
* Version numbers (CallingProgramVersion) (x,y,z):
* x = version number of the model
* y = version number of the GUI
* z = version number of the database
1.1.1-beta      CallingProgramVersion
Hourly          OptInp     ! Option for hourly or daily input data (Hourly, Daily)
* Option to set output time step (OptDelTimPrn):
* (Hour, Day, Decade, Month, Year, Automatic, Other)
* Automatic = length of simulation period
* Other      = user defined
Hour           OptDelTimPrn
*=> If: OptDelTimPrn = Other
1              DelTimPrn  ! Output time step (d) [0.0 - length simulation period]
*<=           ! Integer value required
No            PrintCumulatives ! Specify whether fluxes should be cumulated over
*
               the entire simulation period (Yes , No)
* Hydrology simulation option (OptHyd):
* Only        = Runs only hydrology
* OnLine      = Runs hydrology and substance
* OffLine     = Assumption the hydrology has been run,runID.hyd file must be present
* Automatic   = TOXSWA checks if the hydrology file (runID.hyd) exists. Then the
*
               hydrology simulation is skipped
OnLine        OptHyd
OnLine        OptTem
* Time step substance simulation options (OptTimStp):
* Input       = User defined
* Calc        = Calculated by TOXSWA
Calc          OptTimStp
*=> If: OptTimStp = Input
600 MaxTimStpWat (s) ! Maximum calculation time step in water layer [0.001 - 3600]
600 MaxTimStpSed (s) ! Maximum calculation time step in sediment [0.001 - 3600]
900 TimStpHyd (s) ! Calculation time step for hydrology [0.001 - 3600]
Yes          OptScreen  ! Option to show output on screen [Yes, No]

```

```

*-----
* Section 2: Waterbody
*-----
Netherlands      Location      ! Name of the location
greenhouse_ditch WaterbodyID  ! ID of the water body
* Table WaterBody
* Len            = Length (m) [0.1 - 10000]
* NumSeg         = Number of segments (-) [1 - 1000]
* WidWatSys      = Width of the bottom of water system (m) [0.1 - 100]
* SloSidWatSys   = Side slope of the water system (-) [0.001 - 2]
* DepWatDefPer   = Water depth defining perimeter for exchange between water layer
*                and sediment (m) [0 - lowest water depth]
Table WaterBody
Len  NumSeg  WidWatSys  SloSidWatSys  DepWatDefPer  DepWatSysBot
(m)  (-)     (m)         (-)           (m)           (m)
150   15      1.88        1.20          0.1           0.82
EndTable
11.0   ConSus (g.m-3)      ! Concentration of suspended solids
! [1.0 - 100000]
0.09   CntOmSusSol (kg.kg-1) ! Mass ratio of organic matter in suspended solids
! [0.0 - 1.0]
0.0    AmaMphWatLay (g.m-2) ! Dry weight of macrophyte biomass per m2 bottom
! [0.0 - 1000]
*-----
* Section 3: Hydrology: general
*-----
WaterCourse OptWaterSystemType ! Option for selecting the water system type
! [Pond, WaterCourse]
Variable    OptFloWat          ! Option for water flow [Constant, Variable]
*=> if: OptWaterSystemType = WaterCourse
Fischer     OptDis             ! Option for selecting dispersion method [Fischer,
Input]
*-----
* Section 3a: Constant water flow
*-----
* if: OptFloWat = Constant
*1.0        DepWat (m)          ! Water depth [0.001|10.0]
*100.0      VelWatFlwBas (m.d-1) ! Flow velocity [-100000.0|100000.0]
*-----
* Section 3b: Variable flow: pond
*-----
* if: OptFloWat = Variable and OptWaterSystemType = Pond
*0.45       AreaSurPndInp (ha) ! Size of area surrounding the pond [0.0|100.0]
* if: OptFloWat = Variable and OptWaterSystemType = Pond
*         and CallingProgram = FOCUS
*3.189      QBasPndInp (m3.d-1) ! Base flow, i.e. inflow into pond [0.0|50.0]
*0.5        HgtCrePnd (m)       ! Height of the weir crest [0.1|5.0]
*0.5        WidCrePnd (m)       ! Width of the weir crest [0.01|10.0]
* if: OptFloWat = Variable and OptWaterSystemType = Pond
*         and CallingProgram = FOCUS and Opt = Runoff
*0.6        AreaErsSurPndInp (ha) ! Size of the eroding area around the pond
* if: OptFloWat = Variable and OptWaterSystemType = Pond
*         and CallingProgram = CHINATOXSWA
*0.5        DepWatIni (m)       ! Initial water depth [0.001|10.0]
*1.0        DepPnd (m)          ! Depth of the pond [0.001|10.0]
*0.01       CofRatSpgInp (d-1) ! Percolation resistance of the sediment layer

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```

*0.5      DepWatSpgMin (m)    ! Depth water layer below which percolation does not
                                   ! occur [0.0|5.0]

*-----
* Section 3c: Variable flow: watercourse
*-----

*=> if: OptFloWat = Variable and OptWaterSystemType = WaterCourse
100.0     WidFldLoaInp (m) ! Width of the field [0.0 - 1000.0]
0.0       SloBotWatCrS (-) ! Slope bottom watercourse []
0.16      HgtCreWatCrS (m) ! Hight crest of the weir []
0.50      WidCreWatCrS (m) ! Width crest of the weir []
400.      DstWeiWatCrS (m) ! Distance begin watercourse to weir []
*==> if: CallingProgram = GEM
1.0       AreaPntInp (ha) ! Area of the greenhouses
Westland_D FilSOBEK      ! File with fluxes upstream boundary
Soil_bound OptSys       ! Greenhouse system [Soilles, Soil_bound]
*<==
0.        AreaUpsWatCrSInp (ha)
*-----
* Section 4: Sediment section
*-----

Ditch     SedimentTypeID ! Name of sediment type
* Table SedimentProfile
* ThiHor = thickness of horizon []
* NumLay = number of layers in horizon [1,]
table SedimentProfile
ThiHor NumLay
(m)
0.004    4
0.006    3
0.01     2
0.03     3
0.02     1
0.03     1
end_table
Input     OptSedProperties ! Option sediment properties [Input, Calc]
* table specifying SedimentProperties for each horizon:
* Nr      = number horizon []
* Rho     = bulk density [100 - 2000]
* CntOm   = organic matter mass content [0.0 - 1.0]
* ThetaSat = saturated water content [0.1 - 0.95]
* CofDifRel = relative diffusion coefficient [0.0 - 1.0]
table horizon SedimentProperties
Nr      Rho      CntOm      ThetaSat  CofDifRel
      (kg.m-3)  (kg.kg-1)  (m3.m-3)  (-)
1       800.0    0.09      0.68      0.560
2       800.0    0.09      0.68      0.560
3       800.0    0.09      0.68      0.560
4       800.0    0.09      0.68      0.560
5       800.0    0.09      0.68      0.560
6       800.0    0.09      0.68      0.560
end_table
0.       FlwWatSpg      (m3.m-2.d-1)    ! Rate of percolation through the sediment
* table DispersionLength for each horizon
* Nr      = Horizon number []
* LenDisSedLiq = Dispersion length of solute in liquid phase [0.05 - 1.0]

```

```

table horizon DispersionLength
Nr      LenDisSedLiq
        (m)
1       0.015
2       0.015
3       0.015
4       0.015
5       0.015
6       0.015
end_table
-----
* Section 5: Weather section
-----
DeBilt MeteoStation  ! Name of the *.met file with meteo data
Monthly OptMetInp
* if: OptMetInp = Hourly or Daily
*52.00  LocLat (Degrees)  ! Latitude of meteostation
*-4.00  LocLong (Degrees) ! Longitude of meteostation
*1.0    TimZone (-)      ! Time zone
*20.00  FacWatTur1 (W.m-2) ! Turbidity factor a1
*20.00  FacWatTur2 (W.m-2) ! Turbidity factor a2
*-0.75  FacCldB1 (-)     ! Cloud contribution factor b1
*3.4    FacCldB2 (-)     ! Cloud contribution factor b2
*70.00  FacClcC1 (W.m-2) ! Cloud contribution factor c1
*0.00   FacClcC2 (W.m-2) ! Cloud contribution factor c2
*1.50   MetLvlRef (m)    ! Reference level meteo measurements
*10.00  MetLvlObs (m)    ! Height of meteo measurements
-----
* Section 6: Substance section
-----
EXGE1      SubstanceName
table compounds
EXGE1
end_table
* Table parent-daughter relationships transformation in water (FraPrtDauWat):
* Column 1: fraction formed from parent into daughter
* Column 2: name of parent
* Column 3: name of daughter
table FraPrtDauWat (mol.mol-1)
end_table
* Table parent-daughter relationships transformation in sediment (FraPrtDauSed):
* Column 1: fraction formed from parent into daughter
* Column 2: name of parent
* Column 3: name of daughter
table FraPrtDauSed (mol.mol-1)
end_table
*----- Parent: EXGE1 -----
255.7      MolMas_EXGE1 (g.mol-1)  ! Molar mass [10.0 - 10000]
7.         DT50WatRef_EXGE1 (d)     ! Half-life transformation in water
          ! [0.1 - 100000]
20.        TemRefTraWat_EXGE1 (C)   ! Temperature at which half-life was measured
          ! [5.0 - 30]
1000.     DT50SedRef_EXGE1 (d)     ! Half-life transformation in sediment
          ! [0.1 - 100000]
20.        TemRefTraSed_EXGE1 (C)   ! Temperature at which half-life was measured
          ! [5.0 - 30]
65.4      MolEntTraWat_EXGE1 (kJ.mol-1) ! Molar activation enthalpy of transformation in water
          ! [0.0 - 200]

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```

65.4          MolEntTraSed_EXGE1 (kJ.mol-1) ! Molar activation enthalpy of
transformation in sediment
! [0.0 - 200]
131.          KomSed_EXGE1 (L.kg-1)          ! Coefficient of equilibrium sorption in
! sediment [0.0 - 10000000]
1.           ConLiqRefSed_EXGE1 (mg.L-1)    ! Reference concentration in liquid
phase in
! sediment [0.001 - 100]
0.9          ExpFreSed_EXGE1 (-)           ! Freundlich exponent in sediment [0.1 - 2]
131.          KomSusSol_EXGE1 (L.kg-1)      ! Coefficient of equilibrium sorption
suspended
! solids [0.0 - 10000000]
1.           ConLiqRefSusSol_EXGE1 (mg.L-1) ! Reference concentration in liquid phase
! suspended solids [0.001 - 100]
0.9          ExpFreSusSol_EXGE1 (-)        ! Freundlich exponent suspended solids[0.1 - 2]
0.           CofSorMph_EXGE1 (L.kg-1)      ! Coefficient for linear sorption on
macrophytes
! [0.0 - 20000]
4.E-10       PreVapRef_EXGE1 (Pa)          ! Saturated vapour pressure of substance
! [0.0 - 200000]
20.          TemRefVap_EXGE1 (C)           ! Temperature of reference at which the
saturated
! vapour pressure was measured [0.0 - 40]
95.          MolEntVap_EXGE1 (kJ.mol-1)    ! Molar enthalpy of the vaporization
process
! [-200 - 200]
613.         SlbWatRef_EXGE1 (mg.L-1)      ! Water solubility of substance
! [0.001 - 1000000]
20.          TemRefSlb_EXGE1 (C)           ! Temperature of reference at which the
water
! solubility was measured [0.0 - 40]
27.          MolEntSlb_EXGE1 (kJ.mol-1)    ! Molar enthalpy of the dissolution
! [-200 - 200]
4.3E-5       CofDifWatRef_EXGE1 (m2.d-1)  ! Reference diffusion coefficient in
water
! [0.0 - 200]
*-----
* Section 7: Management section
*-----
* Loading options (OptLoa):
* PEARL      = drainage calculated by PEARL
GEM          OptLoa
GEM ApplicationScheme ! Name of the applicaton scheme
* Table loadings
* Column 1: Date of application, relevant if OptLoa = 'DriftOnly', otherwise
*           the date is a dummy values
* Column 2: Type of loading (-)
* Column 3: Drift deposition (mg.m-2) []
* Column 4: Start of stretch of watercourse loaded by all loading types (m) []
* Column 5: End of stretch of watercourse loaded by all loading types (m)[]
table Loadings
end_table
*==> If: PreVapRef of parent at 20 C > 0.01 Pa
0.0          FraAtmDepCum24h (-)          ! Cumulative fraction atmospheric deposition in 24 h
*<==
No           OptUpsInp (-) ! Option for loading on upstream catchment (Yes, No)
0.0          ConSysWatIni (g.m-3) ! Initial concentration in water layer
0.0          ConAir (kg.m-3) ! Concentration of the substance in air
0.0          ConWatSpg (g.m-3) ! Concentration in incoming seepage water
* Table initial substance content in sediment (CntSysSedIni)
* Column 1: Depth in sediment (m)
* Column 2: Substance content (mg.kg-1)
table interpolate CntSysSedIni (mg.kg-1)
end_table

```

Annex 5 Example assessment reports

Assessment report soilless - surface water (Example project 1- example assessment 1).

Assessment report: GEM 1.1.1

General assessment information

Report generated on : 19-12-2014 10:39:56
Project ID : 1
Assessment ID and Caption : 1 Example assessment 1, (Application of EXGE1 with nutrient solution in cut flowers)
Cultivation - assessment type : Soilless - surface water
Substance code : EXGE1
Substance name : GEM example substance for soil-bound SW and soilless
Selected Crop from the DTG list : Cut flowers

Application scheme:

Nr	Application type	Application date	Dosage (kg/ha)	Depth (m)	Fraction intercepted (-)
1	With nutrient solution	15-4-2001	0.84	NA	NA

Model versions

GEM version : 1.1.1
Build date : 04-Dec-2014
Database version : 1
SPIN version : SPIN (Substances Plug IN) 2.2
WATERMODEL version : 1.0
SUBSTANCE EMISSION model version : v 1 01
TOXSWA version : 3.3.3
PEARL version : 3.1.5
SWAP version : 3237
Copy rights : Alterra, RIVM, PBL and Wageningen UR Greenhouse Horticulture

Soilless specific

Pots : No

Substance name	End-of-pipe removal fraction
EXGE1	0.00

Summary output of model: WATERMODEL

Basin capacity [m3/ha]: 500
Greenhouse area [ha]: 1
Max Na concentration [mmol/l]: 4
Na uptake [factor of concentration]: 0.001
Illumination [micromol/m2/s]: 200
Na rain water [mmol/l]: 0.1
Na osmosis water [mmol/l]: 0.1
Na tap water [mmol/l]: 1.5
Na ground water [mmol/l]: 0.5

Na surface water [mmol/l]: 0.5
Surface water priority: -
Tapwater priority: 3
Ground water priority: -
Basin priority: 1
Drainperc [%]: 50
System leakage [%]: 1.5
Percentage condens recycled [%]: 80
Osmosis used: True
Osmosis capacity [m3/ha/day]: 25
Daynum osmosis start: 91
Daynum osmosis stop: 237

Summary output of model: SUBSTANCE

```
-----
* SUBSTANCE EMISSION MODEL REPORT: Header
*
* Results from the SUBSTANCE EMISSION MODEL (c) Alterra, WUR Greenhouse Horticulture and RIVM
* SUBSTANCE EMISSION MODEL kernel version : v1.1.1
* SUBSTANCE EMISSION MODEL created on : 06-Nov-2014
*
* SUBSTANCE EMISSION MODEL was called from : Greenhouse_Emission_Model_1.0
* Working directory : D:\UserData\GEM\Projects\1\1\SUBSTANCE
* Run ID : 1
* Input file generated on : 17-Dec-2014 17:22:22
*-----
*-----
* Waterflux file: rose
*-----
* Number of substances : 1
* Parent substance : EXGE1
* Application scheme : GEM
*
* End of SUBSTANCE EMISSION MODEL REPORT: Header

* SUBSTANCE EMISSION MODEL REPORT: GEM
*
* Start date : 01-Jan-2000
* End date : 01-Jan-2007
*-----
*
* NumApp 7
* Nr Start of application End of application Dosage (kg ha-1) application type
* 1 15-Apr-2000 00:00:00 15-Apr-2000 02:00:00 0.8400 application with nutrient solution
* 2 15-Apr-2001 00:00:00 15-Apr-2001 02:00:00 0.8400 application with nutrient solution
* 3 15-Apr-2002 00:00:00 15-Apr-2002 02:00:00 0.8400 application with nutrient solution
* 4 15-Apr-2003 00:00:00 15-Apr-2003 02:00:00 0.8400 application with nutrient solution
* 5 15-Apr-2004 00:00:00 15-Apr-2004 02:00:00 0.8400 application with nutrient solution
* 6 15-Apr-2005 00:00:00 15-Apr-2005 02:00:00 0.8400 application with nutrient solution
* 7 15-Apr-2006 00:00:00 15-Apr-2006 02:00:00 0.8400 application with nutrient solution
```

```

* Substance 1 EXGE1
* Substance properties:
* Molar mass (g.mol-1) : 255.7
* Saturated vapour pressure (Pa) : 0.4E-09; measured at (C) 20.0
* Solubility in water (mg.L-1) : 0.6E+03; measured at (C) 20.0
* Half-life in tanks (d) : 1000.0; measured at (C) 25.0
* Selectivity factor for pesticide uptake (-) : 0.4
* coef. for equilibrium sorption on organic matter (m3.kg-1) : 0.1
*
* Important mass fluxes (kg ha-1) of substance EXGE1
*-----
* yr Identifier Applied Transformed Uptake Discharged to surface water
2000 BalMasWat_EXGE1 0.840E+00 0.684E-02 0.674E+00 0.113E+00
2001 BalMasWat_EXGE1 0.840E+00 0.601E-02 0.661E+00 0.127E+00
2002 BalMasWat_EXGE1 0.840E+00 0.667E-02 0.677E+00 0.109E+00
2003 BalMasWat_EXGE1 0.840E+00 0.687E-02 0.707E+00 0.772E-01
2004 BalMasWat_EXGE1 0.840E+00 0.658E-02 0.722E+00 0.610E-01
2005 BalMasWat_EXGE1 0.840E+00 0.624E-02 0.667E+00 0.121E+00
2006 BalMasWat_EXGE1 0.840E+00 0.644E-02 0.676E+00 0.111E+00
*
* END OF SUBSTANCE EMISSION MODEL REPORT: GEM
*-----
* The run time was 4 minutes and 0 seconds

* Summary output of model: TOXSWA
*-----
* TOXSWA REPORT: Header
* Results from the TOXSWA model (c) Alterra
* TOXSWA model version : 3.3.3-R
* TOXSWA created on : 06-Nov-2014
*
* Working directory : D:\UserData\GEM\Projects\1\1\TOXSWA
* Run ID : 1
* Input file generated on : 17-12-2014
*-----
* Scenario : Netherlands
* Meteo Station : DeBilt
* Substance : EXGE1
* Flow Type : Variable
* Water Body Type : greenhouse_ditch
* Simulation Period : 01-Jan-2000 to 31-Dec-2006
*-----
* End of TOXSWA REPORT: Header
* TOXSWA REPORT: Substance properties and substance loadings
*
* Summary for the following substances
*
* Substance 1: EXGE1
* Molar mass (g.mol-1) : 255.7
* Saturated vapour pressure (Pa) : 0.400E-09 measured at (C) : 20.0
* Water solubility (mg.L-1) : 0.613E+03 measured at (C) : 20.0
* Half-life in water (d) : 7.00 measured at (C) : 20.0
* Half-life in sediment (d) : 1000.00 measured at (C) : 20.0
* Kom susp.solids (coef. for sorption on organic matter) (L.kg-1) : 131.00
* Freundlich exponent (-) : 0.90
* Kom sediment (coef. for sorption on organic matter) (L.kg-1) : 131.00
* Freundlich exponent (-) : 0.90
* Kmp (coef. for sorption on macrophytes-dry weight) (L.kg-1) : 0.00

```

```

* End of TOXSWA REPORT: Substance properties and substance loadings

* TOXSWA REPORT: Target percentiles water layer
* Start date simulation : 01-Jan-2000
* End date simulation   : 31-Dec-2006
*
* Time window for selecting the maximum concentration:
* Evaluation period
* Start      End
01-Jan      31-Dec

* Percentile summary for substance EXGE1
* -----
* Period      Date of      Maximum substance
* number      maximum      concentration in water
*                               (ug/L)
* -----
1      20-Apr-2000      382.3
2      24-Apr-2001      292.7
3      22-Apr-2002      597.9
4      11-May-2003      143.3
5      18-Apr-2004      413.1
6      26-Apr-2005      658.7
7      23-Apr-2006      887.5
* The 50 percentile peak concentration of EXGE1 is      413.1 ug/L

* End of TOXSWA REPORT: Target percentiles water layer

* TOXSWA REPORT: Time weighted average exposure concentrations (TWA) water layer selected year
* Targets:
* TWA7      TWA period: 7.0 d Time window Start date: 01-Jan End date: 31-Dec
* TWA21     TWA period: 21.0 d Time window Start date: 01-Jan End date: 31-Dec

* Target  TWA period  Maximum TWA      TWA
*                               Start      (ug/L)
* -----
* Results for substance: EXGE1
TWA7      7.00      10-May-2004-15h00      121.7
TWA21     21.00     03-May-2004-16h30      76.91
*

* End of TOXSWA REPORT: Time weighted average exposure concentrations (TWA) water layer
selected year

* TOXSWA REPORT: Project_Summary
* Report_type      Percentile
* Run_Id           1
* Location         Netherlands
* Meteo_station    DeBilt
* Substance        EXGE1
* Result_EXGE1    413.1 ug/L

* End of TOXSWA REPORT: Project_Summary

```

Assessment report: GEM 1.1.1

General assessment information

Report generated on : 17-12-2014 16:21:21
Project ID : 2
Assessment ID and Caption : 3 Example assessment 3, (Application of EXGE1 to the soil surface in cut flowers)
Cultivation - assessment type : Soil-bound - surface water
Substance code : EXGE1
Substance name : GEM example substance for soil-bound SW and soilless
Selected Crop from the DTG list : Cut flowers

Application scheme:

Nr	Application type	Application date	Dosage (kg/ha)	Depth (m)	Fraction intercepted (-)
1	To the soil surface	20-6-2001	0.65	NA	NA

Model versions

GEM version : 1.1.1
Build date : 04-Dec-2014
Database version : 1
SPIN version : SPIN (Substances Plug IN) 2.2
WATERMODEL version : 1.0
SUBSTANCE EMISSION model version : v 1 01
TOXSWA version : 3.3.3
PEARL version : 3.1.5
SWAP version : 3237
Copy rights : Alterra, RIVM, PBL and Wageningen UR Greenhouse Horticulture

Summary output of model: PEARL

```
* -----  
* PEARL REPORT: Header  
* Results from the PEARL model (c) Alterra, PBL and RIVM  
* PEARL kernel version : 3.1.5  
* SWAP kernel version : swap3237  
* PEARL created on : 12-Nov-2014  
*  
* PEARL was called from : GEM, version 1.1.1  
* Working directory : D:\UserData\GEM\Projects\2\3\PEARL  
* Run ID : 3  
* Input file generated on : 17-12-2014  
* -----  
*
```

```

Location          : Bleiswijk
* Meteo station   : Rotterdam
* Soil type       : SandyClay
* Crop calendar   : STANDARD
* Substance       : EXGE1
* Application scheme : ApplicationScheme_GEM
* Deposition scheme : No
* Irrigation scheme : Waterstromen
*
* End of PEARL REPORT: Header
* -----
* -----
* PEARL REPORT: Drainage
* Start date      : 01-Jan-1981
* End date        : 31-Dec-2006
* Annual application to the soil surface at 20-Jun; dosage = 0.6500 kg.ha-1

* Drainage summary for the following compounds:
* Compound 1 EXGE1
* Molar mass (g.mol-1) : 255.7
* Saturated vapour pressure (Pa) : 0.400E-09; measured at (C) 20.0
* Solubility in water (mg.L-1) : 613. ; measured at (C) 20.0
* Half-life (d) in soil : 117.7; measured at (C) 20.0
* Kom (coef. for sorption on soil organic matter) (L.kg-1) : 131.0
* KF (overall sorption coefficient of the soil target layer) (L.kg-1) : 5.96
* Freundlich exponent (-) : 0.90
* Plant uptake factor (-) : 0.50
* Summary for the tile drainage system:
* -----
* Rank Identifier Percent DateMax ConLiqMax FlvLiqMax
* (%) (ug.L-1) (mm.d-1)
1 Drain1_EXGE1 2.50 17-Aug-1991 0.2047176 1.4930000
2 Drain1_EXGE1 7.50 18-Aug-1998 0.2054727 1.4750000
3 Drain1_EXGE1 12.50 05-Jul-1987 0.2736854 2.4140000
4 Drain1_EXGE1 17.50 05-Jul-2001 0.2745195 1.7660000
5 Drain1_EXGE1 22.50 05-Jul-1997 0.2745353 2.1380000
6 Drain1_EXGE1 27.50 05-Jul-1989 0.2767893 1.7390000
7 Drain1_EXGE1 32.50 05-Jul-2003 0.2815860 1.6780000
8 Drain1_EXGE1 37.50 10-Aug-2002 0.2818407 1.2910000
9 Drain1_EXGE1 42.50 05-Jul-2006 0.2832858 2.0430000
10 Drain1_EXGE1 47.50 17-Aug-1999 0.2833449 1.2010000
11 Drain1_EXGE1 52.50 09-Aug-1990 0.2837240 1.1100000
12 Drain1_EXGE1 57.50 05-Jul-1993 0.2865459 1.9210000
13 Drain1_EXGE1 62.50 04-Jul-1992 0.2865487 1.9240000
14 Drain1_EXGE1 67.50 04-Jul-2000 0.2874228 2.0290000
15 Drain1_EXGE1 72.50 04-Jul-2005 0.2901577 1.9820000
16 Drain1_EXGE1 77.50 04-Jul-1996 0.2921518 1.5870000
17 Drain1_EXGE1 82.50 10-Aug-1994 0.2930310 0.9540000
18 Drain1_EXGE1 87.50 04-Jul-2004 0.2945339 1.4650000
19 Drain1_EXGE1 92.50 17-Aug-1995 0.2947116 0.9890000
20 Drain1_EXGE1 97.50 04-Jul-1988 0.3067675 1.6640000
* End of PEARL REPORT: Drainage
* -----

```

Summary output of model: TOXSWA

```
-----
* TOXSWA REPORT: Header
* Results from the TOXSWA model (c) Alterra
* TOXSWA model version : 3.3.3-R
* TOXSWA created on : 06-Nov-2014
*
* Working directory : D:\UserData\GEM\Projects\2\3\TOXSWA
* Run ID : 3
* Input file generated on : 17-12-2014
* -----
*
* Scenario : Netherlands
* Meteo Station : DeBilt
* Substance : EXGE1
* Flow Type : Variable
* Water Body Type : greenhouse_ditch
* Simulation Period : 01-Jan-2000 to 31-Dec-2006
* -----
*
* End of TOXSWA REPORT: Header

* TOXSWA REPORT: Substance properties and substance loadings
*
* Summary for the following substances
*
* Substance 1: EXGE1
* Molar mass (g.mol-1) : 255.7
* Saturated vapour pressure (Pa) : 0.400E-09 measured at (C) : 20.0
* Water solubility (mg.L-1) : 0.613E+03 measured at (C) : 20.0
* Half-life in water (d) : 7.00 measured at (C) : 20.0
* Half-life in sediment (d) : 1000.00 measured at (C) : 20.0
* Kom susp.solids (coef. for sorption on organic matter) (L.kg-1) : 131.00
* Freundlich exponent (-) : 0.90
* Kom sediment (coef. for sorption on organic matter) (L.kg-1) : 131.00
* Freundlich exponent (-) : 0.90
* Kmp (coef. for sorption on macrophytes-dry weight) (L.kg-1) : 0.00
*
* End of TOXSWA REPORT: Substance properties and substance loadings

* TOXSWA REPORT: Target percentiles water layer
* Start date simulation : 01-Jan-2000
* End date simulation : 31-Dec-2006
*
* Time window for selecting the maximum concentration:
* Evaluation period
* Start End
01-Jan 31-Dec
```

```

* Percentile summary for substance EXGE1
* -----
* Period      Date of      Maximum substance
* number      maximum      concentration in water
*                               (ug/L)
* -----
1      11-Aug-2000      0.2350
2      06-Jul-2001      0.1807
3      19-Aug-2002      0.2274
4      11-Jul-2003      0.2093
5      06-Aug-2004      0.1899
6      20-Aug-2005      0.2275
7      11-Jul-2006      0.2165
* The 90 percentile peak concentration of EXGE1 is      0.2335 ug/L

* End of TOXSWA REPORT: Target percentiles water layer

* TOXSWA REPORT: Time weighted average exposure concentrations (TWA) water layer selected year
* Targets:
* TWA7      TWA period: 7.0 d Time window Start date: 01-Jan End date: 31-Dec
* TWA21     TWA period: 21.0 d Time window Start date: 01-Jan End date: 31-Dec

* Target  TWA period  Maximum TWA      TWA
*                               Start      (ug/L)
* -----
* Results for substance: EXGE1
TWA7      7.00      05-Aug-2000-04h30      0.2068
TWA21     21.00     05-Aug-2000-22h30     0.1590
*

* End of TOXSWA REPORT: Time weighted average exposure concentrations (TWA) water layer
selected year

* TOXSWA REPORT: Project_Summary
* Report_type      Percentile
* Run_Id           3
* Location          Netherlands
* Meteo_station    DeBilt
* Substance        EXGE1
* Result_EXGE1     0.2335 ug/L

* End of TOXSWA REPORT: Project_Summary

```

Assessment report: GEM 1.1.1

General assessment information

Report generated on : 19-12-2014 11:19:22
Project ID : 3
Assessment ID and Caption : 4 Example assessment 4, (Application of EXGE2 to the soil surface in cut flowers)
Cultivation - assessment type : Soil-bound - ground water
Substance code : EXGE2
Substance name : example substance for soil-bound GW
Selected Crop from the DTG list : Cut flowers

Application scheme:

```
-----  
Nr Application type      Application date Dosage (kg/ha) Depth (m) Fraction intercepted (-  
)  
-----  
1 To the soil surface    8-4-2001      0.70          NA          NA  
-----
```

Model versions

GEM version : 1.1.1
Build date : 04-Dec-2014
Database version : 1
SPIN version : SPIN (Substances Plug IN) 2.2
WATERMODEL version : 1.0
SUBSTANCE EMISSION model version : v 1 01
TOXSWA version : 3.3.3
PEARL version : 3.1.5
SWAP version : 3237
Copy rights : Alterra, RIVM, PBL and Wageningen UR Greenhouse Horticulture

Summary output of model: PEARL

```
* -----  
* PEARL REPORT: Header  
* Results from the PEARL model (c) Alterra, PBL and RIVM  
* PEARL kernel version : 3.1.5  
* SWAP kernel version : swap3237  
* PEARL created on : 12-Nov-2014  
*  
* PEARL was called from : GEM,version 1.1.1  
* Working directory : D:\UserData\GEM\Projects\3\4\PEARL  
* Run ID : 4  
* Input file generated on : 19-12-2014  
* -----
```



```

* Location      : Huissen
* Meteo station : Rotterdam
* Soil type     : LightSandyClay
* Crop calendar : STANDARD
* Substance     : EXGE2
* Application scheme : ApplicationScheme_GEM
* Deposition scheme : No
* Irrigation scheme : Waterstromen
*
* End of PEARL REPORT: Header
* -----
* -----
* PEARL REPORT: Leaching
* Start date    : 01-Jan-1981
* End date      : 31-Dec-2006
* Target depth  : 1.00 m
* Annual application to the soil surface at 08-Apr; dosage = 0.7000 kg.ha-1
*
* Leaching summary for compound EXGE2
* Molar mass (g.mol-1) : 200.0
* Saturated vapour pressure (Pa) : 0.100E-09; measured at (C) 20.0
* Solubility in water (mg.L-1) : 50.0 ; measured at (C) 20.0
* Half-life (d) in soil : 20.0; measured at (C) 20.0
* Kom (coef. for sorption on soil organic matter) (L.kg-1) : 100.0
* KF (overall sorption coefficient of the soil target layer) (L.kg-1) : 3.78
* 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) conc in water
*                                           at target depth (ug/L)
* -----
1      01-Jan-1987 31-Dec-1987      301.096      0.0000000      0.000
2      01-Jan-1988 31-Dec-1988      309.009      0.0000000      0.000
3      01-Jan-1989 31-Dec-1989      318.831      0.0000000      0.000
4      01-Jan-1990 31-Dec-1990      307.002      0.0000000      0.000
5      01-Jan-1991 31-Dec-1991      312.583      0.0000000      0.000
6      01-Jan-1992 31-Dec-1992      305.240      0.0000000      0.000
7      01-Jan-1993 31-Dec-1993      305.002      0.0000000      0.000
8      01-Jan-1994 31-Dec-1994      309.867      0.0000000      0.000
9      01-Jan-1995 31-Dec-1995      315.382      0.0000000      0.000
10     01-Jan-1996 31-Dec-1996      310.964      0.0000000      0.000
11     01-Jan-1997 31-Dec-1997      316.095      0.0000000      0.000
12     01-Jan-1998 31-Dec-1998      291.586      0.0000000      0.000
13     01-Jan-1999 31-Dec-1999      329.151      0.0000000      0.000
14     01-Jan-2000 31-Dec-2000      299.406      0.0000000      0.000
15     01-Jan-2001 31-Dec-2001      311.232      0.0000000      0.000
16     01-Jan-2002 31-Dec-2002      289.550      0.0000000      0.000
17     01-Jan-2003 31-Dec-2003      346.568      0.0000000      0.000
18     01-Jan-2004 31-Dec-2004      303.353      0.0000000      0.000
19     01-Jan-2005 31-Dec-2005      315.995      0.0000000      0.000
20     01-Jan-2006 31-Dec-2006      307.905      0.0000000      0.000
* The average concentration of EXGE2 closest to the 90th percentile is 0.000000 ug/L

```

* Leaching summary for compound EXGE3

* Molar mass (g.mol-1) : 150.0
* 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 : 100.0; measured at (C) 20.0
* Kom (coef. for sorption on soil organic matter) (L.kg-1) : 30.0
* KF (overall sorption coefficient of the soil target layer) (L.kg-1) : 1.13
* 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) conc in water
* at target depth (ug/L)
* -----

1	01-Jan-1987	31-Dec-1987	301.096	0.0001127	0.037
2	01-Jan-1988	31-Dec-1988	309.009	0.0001152	0.037
3	01-Jan-1989	31-Dec-1989	318.831	0.0001195	0.037
4	01-Jan-1990	31-Dec-1990	307.002	0.0001152	0.038
5	01-Jan-1991	31-Dec-1991	312.583	0.0001182	0.038
6	01-Jan-1992	31-Dec-1992	305.240	0.0001156	0.038
7	01-Jan-1993	31-Dec-1993	305.002	0.0001157	0.038
8	01-Jan-1994	31-Dec-1994	309.867	0.0001164	0.038
9	01-Jan-1995	31-Dec-1995	315.382	0.0001178	0.037
10	01-Jan-1996	31-Dec-1996	310.964	0.0001205	0.039
11	01-Jan-1997	31-Dec-1997	316.095	0.0001231	0.039
12	01-Jan-1998	31-Dec-1998	291.586	0.0001146	0.039
13	01-Jan-1999	31-Dec-1999	329.151	0.0001273	0.039
14	01-Jan-2000	31-Dec-2000	299.406	0.0001161	0.039
15	01-Jan-2001	31-Dec-2001	311.232	0.0001194	0.038
16	01-Jan-2002	31-Dec-2002	289.550	0.0001114	0.038
17	01-Jan-2003	31-Dec-2003	346.568	0.0001350	0.039
18	01-Jan-2004	31-Dec-2004	303.353	0.0001203	0.040
19	01-Jan-2005	31-Dec-2005	315.995	0.0001269	0.040
20	01-Jan-2006	31-Dec-2006	307.905	0.0001271	0.041

* The average concentration of EXGE3 closest to the 90th percentile is 0.039915 ug/L

* End of PEARL REPORT: Leaching

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

* PEARL REPORT: Project_Summary

* Report_type Leaching
* Result_text Concentration closest to the 90th percentile (ug/L)
* Run_Id 4
* Location Huissen
* Meteo_station Rotterdam
* Soil_type LightSandyClay
* Crop_calendar STANDARD
* Substance EXGE2
* Application_scheme ApplicationScheme_GEM
* Irrigation_scheme Waterstromen
* Deposition_scheme No
* Result_EXGE2 0.000000
* Result_EXGE3 0.039915

* End of PEARL REPORT: Project_Summary

* -----



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Alterra Wageningen UR is the research institute for our green living environment. We offer a combination of practical and scientific research in a multitude of disciplines related to the green world around us and the sustainable use of our living environment, such as flora and fauna, soil, water, the environment, geo-information and remote sensing, landscape and spatial planning, man and society.

The mission of Wageningen UR (University & Research centre) is 'To explore the potential of nature to improve the quality of life'. Within Wageningen UR, nine specialised research institutes of the DLO Foundation have joined forces with Wageningen University to help answer the most important questions in the domain of healthy food and living environment. With approximately 30 locations, 6,000 members of staff and 9,000 students, Wageningen UR is one of the leading organisations in its domain worldwide. The integral approach to problems and the cooperation between the various disciplines are at the heart of the unique Wageningen Approach.

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Alterra Wageningen UR is hét kennisinstituut voor de groene leefomgeving en bundelt een grote hoeveelheid expertise op het gebied van de groene ruimte en het duurzaam maatschappelijk gebruik ervan: kennis van water, natuur, bos, milieu, bodem, landschap, klimaat, landgebruik, recreatie etc.

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