



User manual for SAFE to support the use of the GEM scenarios for cultivations in glasshouses

Version 1.1

F. van den Berg, H. Baveco & E.L. Wipfler

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User manual for SAFE (Select Application date For Evaluation) to support the use of the GEM scenarios for cultivations in glasshouses

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Abstract

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For the assessment of the environmental risks of the use of plant protection products in glasshouse cultivations, exposure scenarios have been developed. These scenarios have been implemented in the Glasshouse Emission Model (GEM). Because the application can cover the entire plant growth cycle, additional guidance was needed to select the application date with the highest Predicted Environmental Concentration for the assessment of leaching to ground water in soil-bound cultivations and that of exposure of aquatic organisms in soilless cultivations. The software tool SAFE (Select Application date For Evaluation) has been developed to assist the user with the selection of the application date. Two variants of this tool have been developed: one for soil-bound cultivations and one for soilless cultivations. The use of both variants is described in this user manual.

Keywords: drainage, groundwater, leaching, pesticide, plant protection product, surface water, soil-bound, soilless, greenhouse, exposure assessment

Referaat

Om de milieurisico's van het gebruik van gewasbeschermingsmiddelen in kasteelten te beoordelen, zijn blootstellingsscenario's ontwikkeld. Deze scenario's zijn geïmplementeerd in het Glasshouse Emission Model (GEM). Omdat de toepassing gedurende de gehele teelt kan plaatsvinden, is een richtlijn nodig voor de selectie van de toepassingsdatum, die resulteert in de hoogst berekende concentratie voor de beoordeling van de uitspoeling naar het grondwater in grondgebonden teelten en de beoordeling van de blootstelling van waterorganismen in substraatteelten. Het SAFE (Select Application date For Evaluation) software-instrument is ontwikkeld om de gebruiker te helpen bij het selecteren van de toepassingsdatum. Twee varianten van het SAFE-model zijn ontwikkeld: een voor grondgebonden teelten en een voor substraatteelten. Het gebruik van beide varianten wordt beschreven in deze gebruikershandleiding.

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Preface

For the evaluation of risks to aquatic organisms and the risk of leaching of plant protection products to groundwater in Dutch greenhouses, exposure scenarios have been developed for soil-bound and soilless cultivations. To support the exposure assessment using these scenarios the GEM (Glasshouse Emission Model) software tool has been developed. Because the exposure scenario is predefined the only data the user has to specify are the input data related to the physico-chemical properties of the compound and the application characteristics. The predicted environmental concentration (PEC) calculate by GEM depends not only on the properties of the compound but also on the date of application. As the aim is to calculate the highest PEC for a specific compound over the application period considered, the date of application should be carefully selected. For some plant protection products the application window can practically cover the entire crop cycle, which raises the problem how to find the application date resulting in the maximum PEC. Therefore, the Dutch Board for the Authorisation of Plant Protection Products and Biocides (Ctgb) has requested the Ministry of Agriculture, Nature and Food Quality for guidance on the selection of the application date in the application of the relevant GEM scenarios for soilless as well as soil-bound cultivations.

In response to the request by Ctgb, the Ministry of Agriculture, Nature and Food Quality has commissioned Wageningen Environmental Research to develop guidance to select the possible application date for the assessment of relevant scenarios in the current version of GEM, i.e. version 3.3.2. Guidance development was done in collaboration with Ctgb to ensure a good connection to daily regulatory assessment practices, which resulted in the software instrument SAFE (Select Application date For Evaluation). There are two variants of this tool: SAFE soil-bound and SAFE soilless.

Erik van den Berg, Hans Baveco & Louise Wipfler

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Summary

In the authorization procedure for the use of plant protection products in glasshouses the Glasshouse Emission Model (GEM) is used to assess the risks of leaching of the active ingredients to ground water in soil-bound cultivations and of exposure of aquatic organisms in soil-bound and soilless cultivations. The GEM model supports the calculation of Predicted Environmental Concentrations based on pre-developed exposure scenarios for either soil-bound or soilless cultivation.

The Predicted Environmental concentration is sensitive to the timing of the application of the plant protection product. In addition, the application period for a specific plant protection product may practically cover the entire crop development cycle. A software tool has been developed to assist the user of the GEM model to find the application date resulting in the maximum PEC.

The software tool SAFE (Select Application date For Evaluation) has two variants, one for the selection of the application date for the groundwater scenario in soil-bound cultivations and another for the selection of the application date for the surface water scenario in soilless cultivations. Each variant has a user-friendly interface and the SAFE model kernel. The user interface offers the user different options to use the SAFE model. On the basis of the selected option, SAFE will generate a number of runs for all required application dates and consecutively start these runs. SAFE makes use of the model kernels of the current GEM version, i.e. version 3.3.2. Once these runs are finished the SAFE Soil-bound or SAFE Soilless model kernel extracts the target output from each run and writes to the SAFE report file the highest PEC and the application date that gives this highest PEC.

Samenvatting

In de toelatingsprocedure voor het gebruik van gewasbeschermingsmiddelen in de glastuinbouw wordt het Glasshouse Emission Model (GEM) gebruikt om het risico op uitspoeling naar het grondwater in grondgebonden teelten en dat van blootstelling van waterorganismen in zowel grondgebonden als substraatteelten te beoordelen. Het GEM-model ondersteunt de berekening van de blootstellingsconcentratie in het milieu op basis van vooraf gedefinieerde scenario's voor hetzij grondgebonden dan wel substraatteelten.

De berekende concentratie in het milieu is gevoelig voor het tijdstip van toediening. Bovendien kan een bepaald gewasbeschermingsmiddel toegepast worden gedurende vrijwel de gehele teeltcyclus. Een software-instrument is ontwikkeld om de gebruiker van het GEM-model te helpen om de datum van toepassing te vinden die in de hoogste berekende waarde van deze concentratie resulteert.

Het SAFE (Select Application date For Evaluation) software-instrument heeft twee varianten: een variant voor de selectie van de toepassingsdatum voor het grondwaterscenario bij de grondgebonden teelten en een andere voor de selectie van de toepassingsdatum voor het oppervlaktewater-scenario bij substraatteelten. Elke variant heeft een gebruikersvriendelijke interface en een SAFE-modelkern. Het interface biedt de gebruiker een aantal opties voor het gebruik van SAFE. Op basis van de gekozen optie maakt SAFE runs aan voor alle gewenste toedieningsdata en stuurt de uitvoering van de runs aan. Bij de berekeningen wordt gebruik gemaakt van de bestaande onderliggende modellen van GEM 3.3.2. Zodra de runs voltooid zijn extraheert SAFE het resultaat van elke run en maakt een rapport met daarin de hoogste de concentratie en de daarbij behorende toedieningsdatum.

1 Introduction

For the assessment of the emission of crop protection products resulting from their use in glasshouses, exposure scenarios have been developed for soilless cultivations and soil-bound cultivations (Van der Linden *et al.* 2015, Wipfler *et al.* 2015). To support the exposure assessment using these scenarios the software tool GEM (Glasshouse Emission Model) has been developed. For soil-bound cultivations the PEARL model is run to assess the leaching of the active substance and its metabolites to groundwater. For soilless cultivations the WATERSTROMEN model, the Substance Emission model and the TOXSWA model are run to calculate the surface water concentrations of the active substance and its metabolites.

For each substance to be assessed data on the properties of the substance have to be specified in the PEARL input file (for SAFE Soil-bound) or the SUBSTANCES input file (SAFE Soilless) as well as application specific data, such as the application date and the dosage. For some crop-compound combinations the application window can be quite large, even covering the whole calendar year. For such compounds the application date has to be selected that results in the highest PEC, i.e. the 90th percentile leaching concentration at 1 m depth for the GEM groundwater scenario for soil-bound cultivations or the highest 50th or 90th percentile surface water concentration¹ for the GEM surface water scenario for soilless cultivations.

In order to support the user determining the application date resulting in the highest Predicted Environmental Concentration (PEC), the SAFE tool has been developed for both soil-bound and soilless cultivations. SAFE is an acronym for Select Application date For Evaluation. The SAFE tool can only be used in combination with GEM version 3.3.2. The installation of this tool is described in Chapter 2. In Chapter 3 the interfaces of the two variants of this tool are presented and their use is explained.

SAFE Soil-bound cultivations

For a successful installation of SAFE Soil-bound, GEM version 3.3.2 has to be installed first. During installation SAFE automatically finds the bin directory of the PEARL and SWAP models, so the user will have no difficulty in executing PEARL model runs when using SAFE. The hydrological model SWAP is fully coupled to the PEARL model. This means that the PEARL model creates all the input files for SWAP, calls the SWAP model and uses the hydrological output of SWAP for the greenhouse soil to calculate the leaching concentration at 1 m depth.

The installation of SAFE starts after clicking on the setup.exe of the installation package. The user is guided throughout the installation procedure. For more detailed information consult the ReadMeDuringInstallation.

Special attention need to be paid by the user to select the output folder. To ensure a proper functioning of the tool, the user should select a local drive and the user should have permission to write output files to this folder.

SAFE Soilless cultivations

SAFE Soilless is installed simply by unpacking SafeSL.zip at the desired location. The zip file contains the program in a single directory, named SAFE-SL. Start the program by double-clicking the executable SafeSL.exe. For convenience, a shortcut can be created linked to SafeSL.exe on the desktop.

SAFE Soilless has been developed in open-source Smalltalk, Pharo 7.0 (<http://pharo.org>) with packages loaded for visualization (Roassal2), handling of csv files (NeoCSV), export of xlsx files (Tabular) and for access to operating system functionality (OSProcess).

¹ The selected percentile depends on the assessment. See for details on which percentile to select the Ctgb website

2 User Guide of SAFE Soil-bound

After starting the SAFE Soil-bound application the main form is shown (See Figure 2.1). In the upper part the locations of the input and output files must be set as well as the location of the Pearl model and SWAP executables to run the GEM 3.3.2 groundwater scenarios. In the lower part of the main screen the input data required to run SAFE Soil-bound are listed.

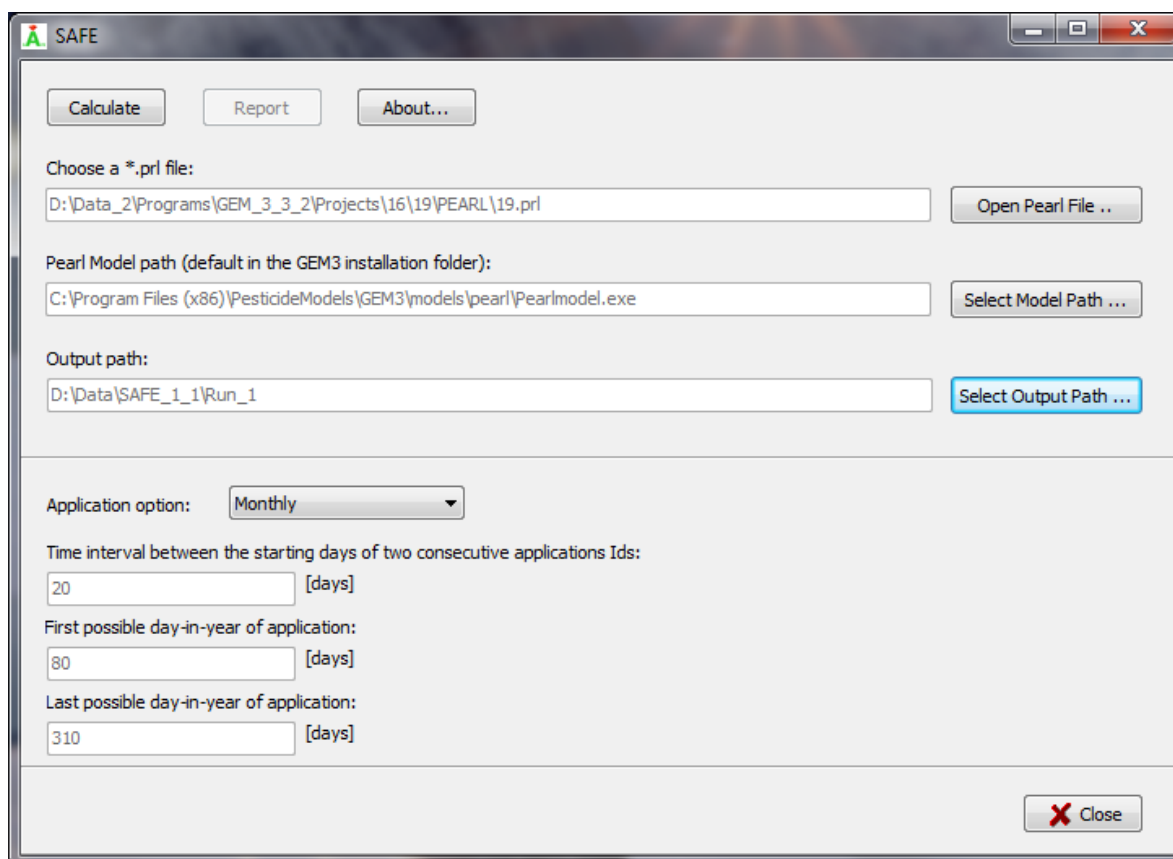


Figure 2.1 The main form of SAFE Soil-bound

2.1 Preparation of input

To prepare an assessment for SAFE Soil-bound the user has to adhere to the following procedure:

1 Click on the button 'Open Pearl file ...' to navigate to the folder with the prl file for the GEM 3.3.2 run to be assessed with SAFE Soil-bound and select the .prl file.

2 Click on the button 'Select output path ...' to navigate to and select a local folder for the output of the SAFE Soil-bound assessment.

As mentioned above, the field with the caption 'Pearl model path' shows the folder in which the Pearlmodel and swap executables have been installed by GEM version 3.3.2. The user does not have to navigate to find the Pearlmodel.exe, as this has already been done during the installation of SAFE Soil-bound.

In the lower part of the main form the user has to specify the application option. This can be either 'Monthly' or 'User Defined'.

If the user selects 'Monthly' no more input data are needed. The application dates in these twelve runs are the 15th of each month. If the application scheme contains more than one application then the first application is set to the 15th of the month; the interval between the other applications is the same as in the PEARL input file created by GEM.

If the user selects the option 'User defined' then the user has to specify the three parameters shown in the lower part of the main screen of SAFE Soil-bound. These are:

- The time interval between the starting days of two consecutive application Ids;
- The first possible day-in-year of the application;
- The last possible day-in-year of the application.

The application Id refers to a specific application scheme as defined in a single run. So the time interval between the starting days of two consecutive application Ids is the time interval as specified in two consecutive runs as created by SAFE.

If the application can be done throughout the year the first day-in-year is day number 1 and the last day-in-year is day number 365.

If the time window is restricted to the period May – June then the first day-in-year is day 121 and the last day-in-year is day 181. A Day-In-Year calendar is included in Annex 2. This can help the user to find quickly the day-in-year number for the first and last possible days of application.

For example, if the application scheme as specified using the GEM v. 3.3.2 interface consists of three applications with an interval between two applications of seven days and the time window of application starts on 1 May then the run for the first application Id has the following application dates:

1-May
8-May
15-May

If the user has specified the time interval between the starting days of two consecutive application Ids to be 3 days, the run for the next application Id has the following application dates:

4-May
11-May
18-May

2.2 Execute application scenarios

The user can start SAFE Soil-bound by clicking on the button 'Calculate' in the upper part of the main screen. Subsequently SAFE will create the pearl input files for all application Ids and run them one after the other. The progress of the runs is shown in the DOS Window, which is shown in Figure 2.2. The application Id is added as a suffix to the AssessmentId for this pearlmodel run in GEM 3.3.2.

In the example shown in Figure 2.2, the assessment Id is 21 and the suffix for this run is '1', being the first of the twelve Pearlmodel runs for the SAFE 'Monthly' application option to be executed in this SAFE Soil-bound assessment.

2.3 About SAFE Soil-bound

The user can also execute a SAFE run created by the SAFE user interface in batch mode. The user has to go to the SAFE output directory. The input files of SAFE for this run, with the extension .ssb, can be found in the folder selected for the SAFE output (see Section 2.1). It is also possible to edit manually the input.ssb file for SAFE Soil-bound.

The .ssb input file contains the following data:

[Path]	BinDir	! Path to executable of PEARL
Monthly	OptApp	! Options are Monthly or UserDefined
20	DelTimAppId (d)	! Time interval between the starting days of two consecutive application Ids
80	DayInYeaAppFirst (d)	! First possible day-in-year of application
310	DayInYeaAppLast (d)	! Last possible day-in-year of application

For example, the user can adjust the first and last days of application. After saving these changes the user can start the run using the modified input by clicking on the SAFE.bat file.

After clicking on the 'About' button information on the software components and the software developers is shown. This screen is shown in Figure 2.4.



Figure 2.4 The 'About' screen of SAFE Soil-bound.

3 User guide of SAFE Soiless

After starting the SAFE Soiless (SAFE_SL) application the main form is shown (See Figure 3.1). All functionality is accessible through buttons on the main screen. Settings and options are specified using input fields and by selecting items from lists. User interface elements are grouped by their functionality: related to project selection (upper part of the window), scenario and assessment definition and scenario execution (middle part) and providing visual feedback (lower part). The definitions of the terms used in SAFE soiless is summarized in Annex 3.

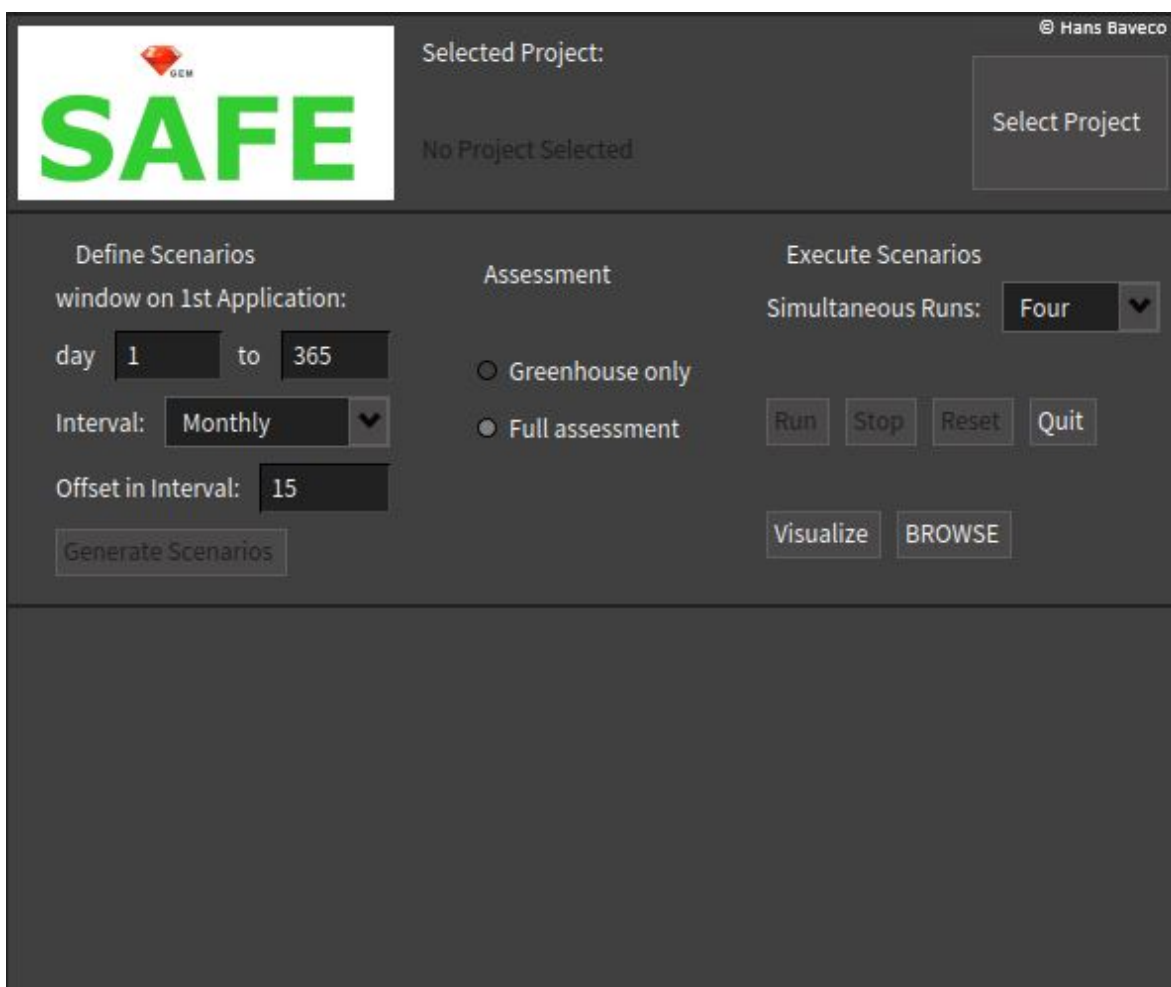


Figure 3.1 The main screen of SAFE Soiless (SAFE_SL)

3.1 Preparation of input

In order to prepare the runs using SAFE_SL the user has to follow the following steps:

- Select a project
- Define scenarios
- Select a run option for the scenarios

After clicking on the 'Select Project'-button a window opens in which the user can select a fully specified assessment created by GEM 3.3.2: a directory containing input and batch files for running the Substrate model and the TOXSWA model, in subdirectories SUBSTANCE and TOXSWA, respectively. This directory will be referred to as the *project directory*. After selection (Figure 3.2), the path of the selected directory

is shown bottom-centre of the top pane. The program will extract all definitions, including the specification of the location of the executables, from this original assessment. Note that no checks are done on the validity of the specifications; therefore the user is advised to select directories of soilless scenario type projects in GEM 3.3.2. In fact, the only aspect of a run in such a project that is modified by SAFE_SL is the section related to application timing in the substrate model input file (*_sub.inp).

To find the assessment you are interested, start up GEM 3.3.2 and go to the assessment you want to analyse in SAFE_SL. Under the tab 'status' you find the path to the directory at the bottom of the window in GEM.

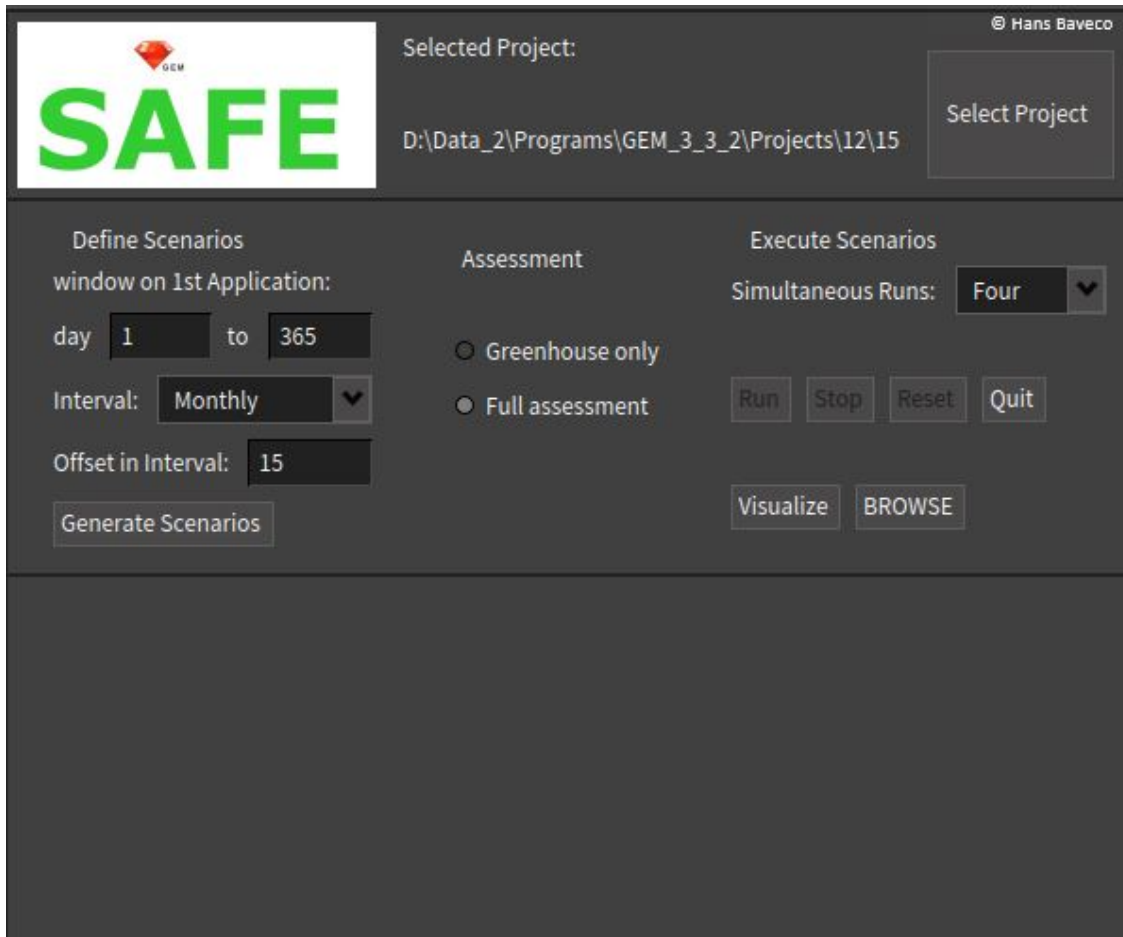


Figure 3.2 Selecting a directory

In step 2 of the procedure the user should select the interval to be used in the analysis. The possible intervals are quarterly, monthly, biweekly, weekly and daily. For a quick-scan over a whole year monthly intervals may suffice. Where needed the user can zoom in and use intervals of e.g. a single day, taking advantage of the option to narrow down the time window (see below).

A time window for the first application can be set to limit the analysis to a specific time of the year, with begin and end day of the time window expressed as a Day-In-Year number (hover the mouse pointer over the field to see the associated date). Default day 1 to 365 are assumed. New edits in the two input fields should be accepted before scenarios can be generated: click on the Enter button after filling in the field. Note that the field turns yellow when the value provided has not yet been saved by SAFE_SL.

The offset of the first application within the selected interval can be set as well. Defaults and maximum allowed values are shown in Table 3.1. When hovering the mouse pointer over the field, the possible range of values for the currently selected interval is shown. Also here a valid offset value should be specified and accepted before scenarios can be generated.

Table 3.1 The default and maximum values for the parameter 'Offset in Interval' for the time interval types in SAFE Soiless.

Interval type	Default value	Maximum value
QUARTERLY	46	90
MONTHLY	15	28
BIWEEKLY	8	14
WEEKLY	4	7
DAILY	1	1

Then, after clicking on the 'Generate Scenarios' button, the scenarios specified are created. Each scenario refers to a complete specification of a Substrate and TOXSWA assessment in GEM 3.3.2., including the definitions of the interval and the offset within the interval. Under the selected project directory a SCENARIOS subdirectory is created to hold all analyses related to the selected project. Under this SCENARIOS directory, each scenario will have its own subdirectory named after the selected interval (QUARTERLY, MONTHLY, BIWEEKLY, WEEKLY or DAILY) with the chosen 'Offset in Interval' appended to the directory name. This directory will be referred to in the following as the *scenario directory*. A standard MS Explorer window can be used to go to the scenario directory, e.g. '..58\SCENARIOS\MONTHLY_15', by clicking the 'BROWSE' button. Each simulation is placed in a subdirectory of the scenario directory, named according to the simulation id. Simulation ids are integers in the range of 1 to N, where 1 refers to the first simulation and N refers to the last simulation. The numbers (ids) of the simulations are 'absolute' and refer to their position in the full time window ranging from day 1 to 365. Hence the directory /SCENARIOS/MONTHLY_15/1 always refers to the simulation with the first application on the 15th of January. This way simulations can be reused when selecting a different time window that overlaps a time window of a previous analysis. Note that (results for) all scenarios defined for the same time interval and offset end up in the same scenario directory. After clicking on the 'Generate Scenarios' button, a representation of the associated simulation runs appears in the lower pane. Blue rectangles represent the simulation runs that are part of the analysis, with a label corresponding to simulation id (Figure 3.3).

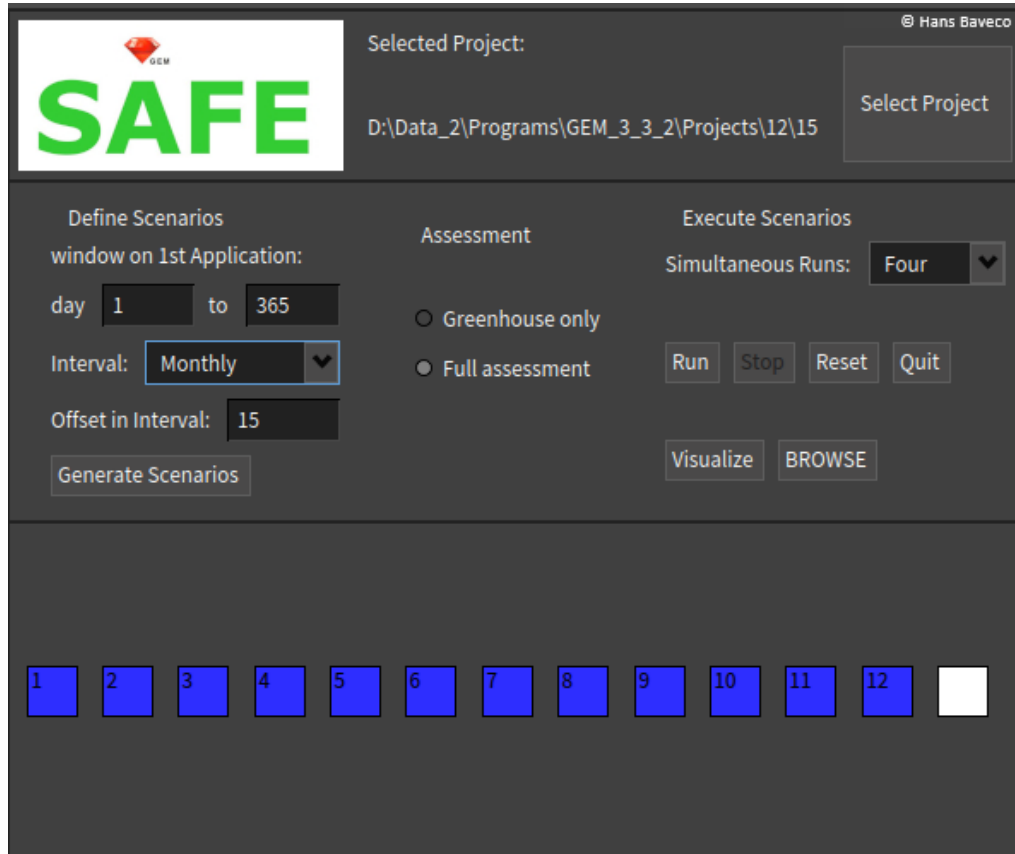


Figure 3.3 The user-interface with the runs created for a monthly application interval

In the third step, the user should choose between a full assessment (SUBSTANCE MODEL and TOXSWA) or an assessment for the SUBSTANCE model only, i.e. 'Greenhouse only'. When the latter is selected, the outcome of the greenhouse simulations can be used afterwards for a full assessment, so the greenhouse simulations will not be repeated.

3.2 Execute application scenarios

After the scenarios have been defined, the runs can be executed directly from the user interface. The user can specify the number of simultaneous runs (parallel processes). Optimally this number matches the number of available cores (or one less). Information on the available number of cores can be obtained by opening a DOS-box (enter 'cmd' in the field at the bottom of the Windows start menu) and typing in the box 'wmic cpu get NumberOfCores'.

After clicking on the 'Run' button, the interface spawns the processes running the simulations in DOS-boxes. It will keep track of the running processes and assure no more than the specified number of runs are simultaneously active. When a simulation is running the corresponding box is shown in red, which is shown in Figure 3.4.

When the simulation is finished the corresponding box will turn into grey. 'Stop' will interrupt and kill the currently running processes. They can be restarted again by clicking on the 'Run' button. Clicking on the 'Reset' button will do the same as clicking on the 'Stop' button, but in addition completely removes the scenario definitions – thus allowing the user to specify a different scenario, or even select a different project to start from. Note that scenarios are only removed from the analysis – associated files located physically on disk are never removed!

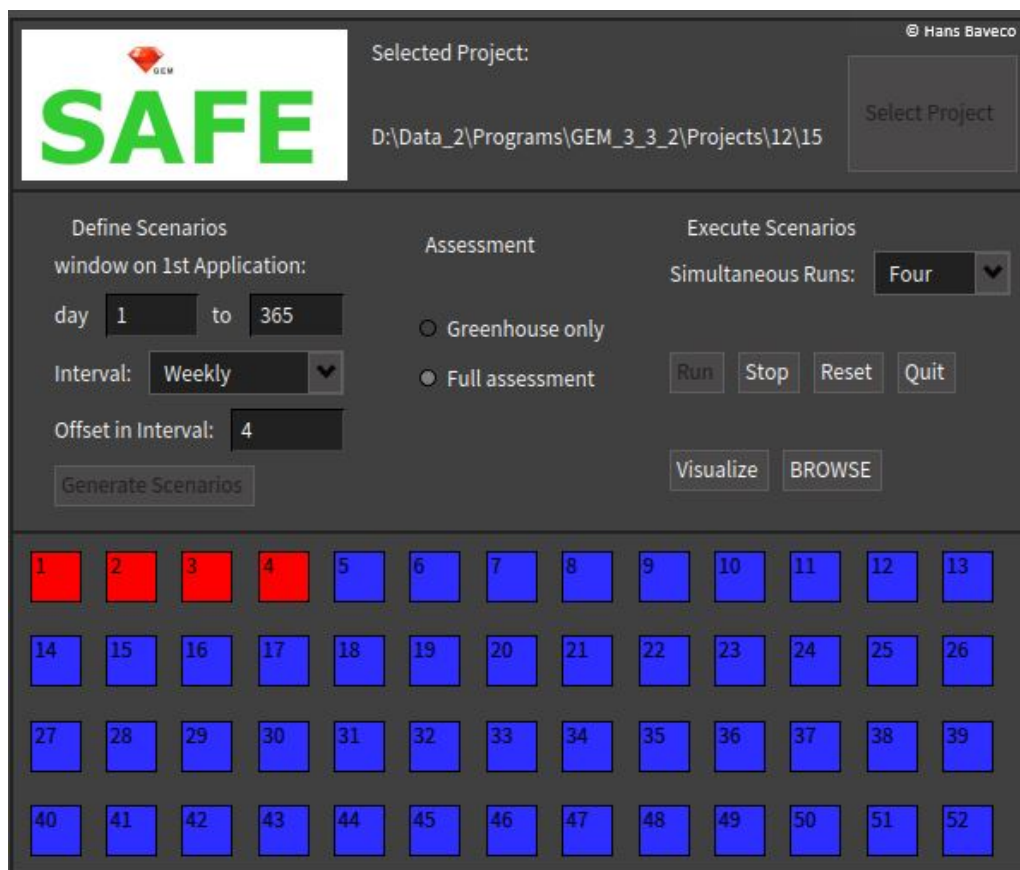


Figure 3.4 The user-interface with the first four simulations of the in total 52 running

When all simulations have finished, the statistics (50-percentiles of annual maximum concentrations in the ditch) are collected and visualized after clicking on the 'Visualize' button. The main graph (Figure 3.5) with the 50-percentiles is displayed in the user interface and exported as .png image to the scenario directory (named TOXSWA REPORT Project_Summary_50-percentile.png).

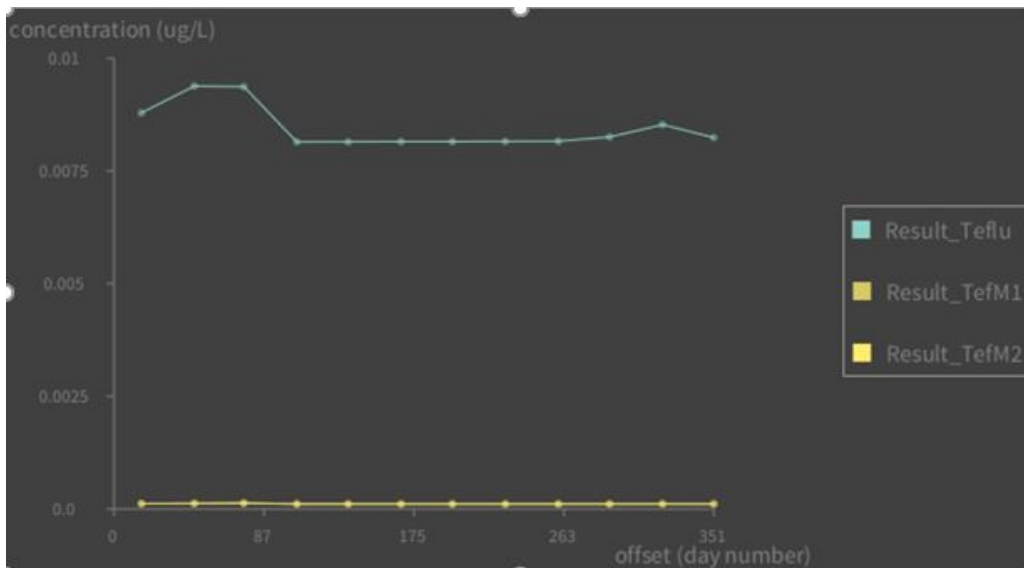


Figure 3.5 The 50-percentile values of annual maximum concentration for a substance and its metabolites, for applications starting halfway the month (analysis with monthly intervals, offset day 15)

Another graph (Figure 3.6) provides an overview of all the annual maximum concentrations and the day in year on which they were observed. The underlying data for these graphs are exported as tab-separated ascii text files and in xlsx-format, to be opened in excel (files named *TOXSWA REPORT Project_Summary_50-percentile* and *datesOfMaxConcColumns*, respectively). The highest TWA values for all the simulations, with the date they were observed, are collected in ascii text files, e.g. *TWA7.txt* and *TWA21.txt*. All output can be found in the corresponding scenario directory (start windows explorer in this directory by clicking on the 'BROWSE' button).

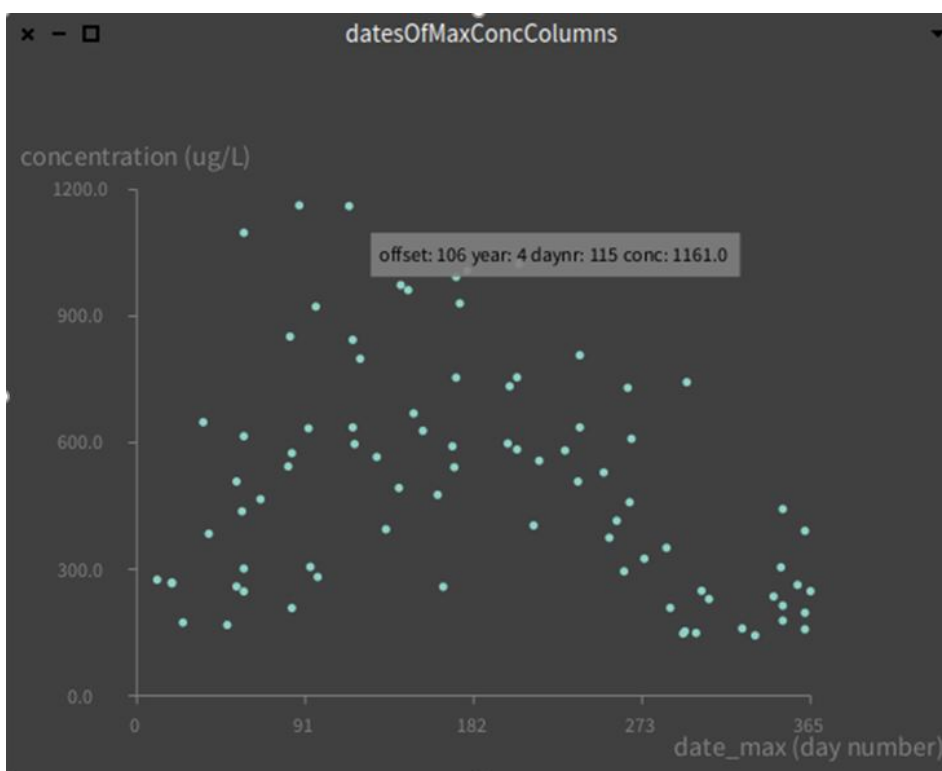


Figure 3.6 All observed (annual) maximum concentrations in the simulations (y-axis) against their day number (x-axis). When hovering the mouse over a data point, a popup shows the associated settings (offset = the day number of first application; year = the simulation year; daynr = the day in year number; conc = the calculated maximum concentration). Note that this information in popups is available in the HTML5 output as well, when opened in an internet browser.

3.3 Tips and Tricks

SAFE_SL specifies Substrate and TOXSWA simulations that differ from the 'parent' project only in their application timing. Once specified, these simulations can also be run outside the user interface, simply by double-clicking the batch files in the simulation directories. SAFE_SL does not remove any created directories or files: clean-up has to be done by the user. When running the scenarios SAFE_SL checks for the presence of the sub.ok and toxswa.ok files. When sub.ok is present, the Substrate model will not be executed. When toxswa.ok is present, the TOXSWA model will not be run. This way results of a previous analysis are not overwritten but instead reused. In case the user wants to force the program to redo previous calculations, he/she should remove either the *.ok file(s), the simulation directory where these ok files are found, or even remove or rename the complete scenario directory (the one that appears when clicking the 'BROWSE' button). Removing simulation or scenario directories will require 'Generate Scenarios' to be run again.

The visualization and creation of the final analysis output (triggered by clicking the 'Visualize' button) is always based on the generated scenarios for the specific window of 1st application, shown in the bottom pane of the interface. This implies that even when more scenarios with their results are present (in scenario directories in the analysis directory) as a result of a previous analysis with different window of 1st application, they will not be included in the present analysis. To incorporate them, generate a new set of scenarios with a wider window of 1st application that encompasses both windows, run them (runs already done will be skipped) and when finished click on the 'Visualize' button. Note that the output files in the analysis directory will always be overwritten when a new analysis is performed involving one or more scenarios in the same analysis directory!

Problems when running the scenarios may have different origins. Although it is unlikely that SAFE_SL will generate invalid specifications of application times in the Substrate and TOXSWA input files, this cannot be excluded completely.

Other origins may be in the handling of the created processes at the level of the operating system. Using the 'stop' and 'run' buttons currently running processes can be killed and restarted. If this does not work properly, quitting and restarting the SAFE_SL program may be the only option left (clicking on 'quit' button). Please note that in such a case already finished simulations will be preserved.

Problems with simulations that are apparently not running may stem from e.g. locations of the Substrate and/or TOXSWA executables that were changed. In most cases, the first step in debugging a problem should be to run the scenario by hand, i.e. navigate to the simulation directory using windows explorer and double-click on the batch file in this directory. To prevent DOS-boxes from closing immediately after finishing, the associated batch file can be opened in a text editor and a PAUSE statement added at the end. This allows the user to read the error message written to the screen and use this information to try to solve the problem.

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Justification

After the introduction of the exposure assessment scenarios in the Dutch authorization procedure for the use of plant protection products in glasshouses, it became clear that additional guidance was needed on the selection of the application date for compounds with a large application window. Following a request for guidance by Ctgb, the Ministry of Agriculture, Nature and Food Quality financed a project to develop guidance on the selection of the application date in the application of the relevant GEM scenarios for soilless as well as soil-bound cultivations.

A draft version of this manual has been commented by Nico Tan from Ctgb. His contribution to the user manual is gratefully acknowledged.

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

Annex 1 Example of SAFE Soil-bound report

```
* -----
* SAFE Soilbound REPORT: Header
* Results from the SAFE Soilbound model (c) WENR
* SAFE Soilbound created on : 12-Sep-2018
* SAFE Soilbound version   : 1.0.3
*
* Working directory       : D:\Data\SAFE_1_1\TestRun
* Run ID                  : 21
* Input file generated on  : 23-04-2019
*
* End of SAFE Soilbound REPORT: Header
* -----
*
* SAFE Soilbound to select application date for groundwater scenario GEM
* for soil-bound cultivations in greenhouses
*
* -----
* Summary of calculations for application dates covering a full calendar year
*
* ApplicationId    PEC80 for each compound; total number of compounds is:  1
*   1              0.9684E-01
*   2              0.9163E-01
*   3              0.7944E-01
*   4              0.4968E-01
*   5              0.3052E-01
*   6              0.2672E-01
*   7              0.2522E-01
*   8              0.3088E-01
*   9              0.3593E-01
*  10              0.4636E-01
*  11              0.6085E-01
*  12              0.7796E-01
*
*
* Sorted data of calculations for application dates covering a full calendar year
* Number Identifier  Percentile  ApplicationId  Leaching concentration (ug/L)
*
*   1  Sub_1         4.17      7    0.2522E-01
*   2  Sub_1        12.50     6    0.2672E-01
*   3  Sub_1        20.83     5    0.3052E-01
*   4  Sub_1        29.17     8    0.3088E-01
*   5  Sub_1        37.50     9    0.3593E-01
*   6  Sub_1        45.83    10    0.4636E-01
*   7  Sub_1        54.17     4    0.4968E-01
*   8  Sub_1        62.50    11    0.6085E-01
*   9  Sub_1        70.83    12    0.7796E-01
*  10  Sub_1        79.17     3    0.7944E-01
*  11  Sub_1        87.50     2    0.9163E-01
*  12  Sub_1        95.83     1    0.9684E-01
*
*
* -----
* SAFE Soilbound Report: Leaching
*
* Results for compound: Sub_1
* The maximum leaching concentration is:    0.9684E-01 ug/L
* This maximum occurs for applicationId:    1
* The first day of application for this applicationId is: 15-Jan
*
* End of SAFE Soilbound Report: Leaching
* -----
```


Annex 2 Day of year calendar

Day in Month	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31
January	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31
February	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59			
March	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90
April	91	92	93	94	95	96	97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120	
May	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144	145	146	147	148	149	150	151
June	152	153	154	155	156	157	158	159	160	161	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180	181	
July	182	183	184	185	186	187	188	189	190	191	192	193	194	195	196	197	198	199	200	201	202	203	204	205	206	207	208	209	210	211	212
August	213	214	215	216	217	218	219	220	221	222	223	224	225	226	227	228	229	230	231	232	233	234	235	236	237	238	239	240	241	242	243
September	244	245	246	247	248	249	250	251	252	253	254	255	256	257	258	259	260	261	262	263	264	265	266	267	268	269	270	271	272	273	
October	274	275	276	277	278	279	280	281	282	283	284	285	286	287	288	289	290	291	292	293	294	295	296	297	298	299	300	301	302	303	304
November	305	306	307	308	309	310	311	312	313	314	315	316	317	318	319	320	321	322	323	324	325	326	327	328	329	330	331	332	333	334	
December	335	336	337	338	339	340	341	342	343	344	345	346	347	348	349	350	351	352	353	354	355	356	357	358	359	360	361	362	363	364	365



Annex 3 Definitions used in SAFE soilless

Scenario	Set of simulations corresponding to the same GEM-soilless cultivation assessment
Simulation	One of the runs of a scenario providing the PEC for one of the created application timings
Interval	The interval between application timing in the different simulations making up the scenario
Offset in interval	Timing of the first application with respect to the first of January (day 1)
Project directory	The directory associated with an assessment (project) in GEM 3.3.2
Scenario directory	The directory associated with a <i>SAFE sl</i> analysis, holding simulation subdirectories
Simulation directory	The directory with the SUBSTRATE and TOXSWA definitions, input and batch files needed for a simulation

Verschenen documenten in de reeks Technical reports van de Wettelijke Onderzoekstaken Natuur & Milieu vanaf 2018

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