Hands-on exercises GEM course February 2016.

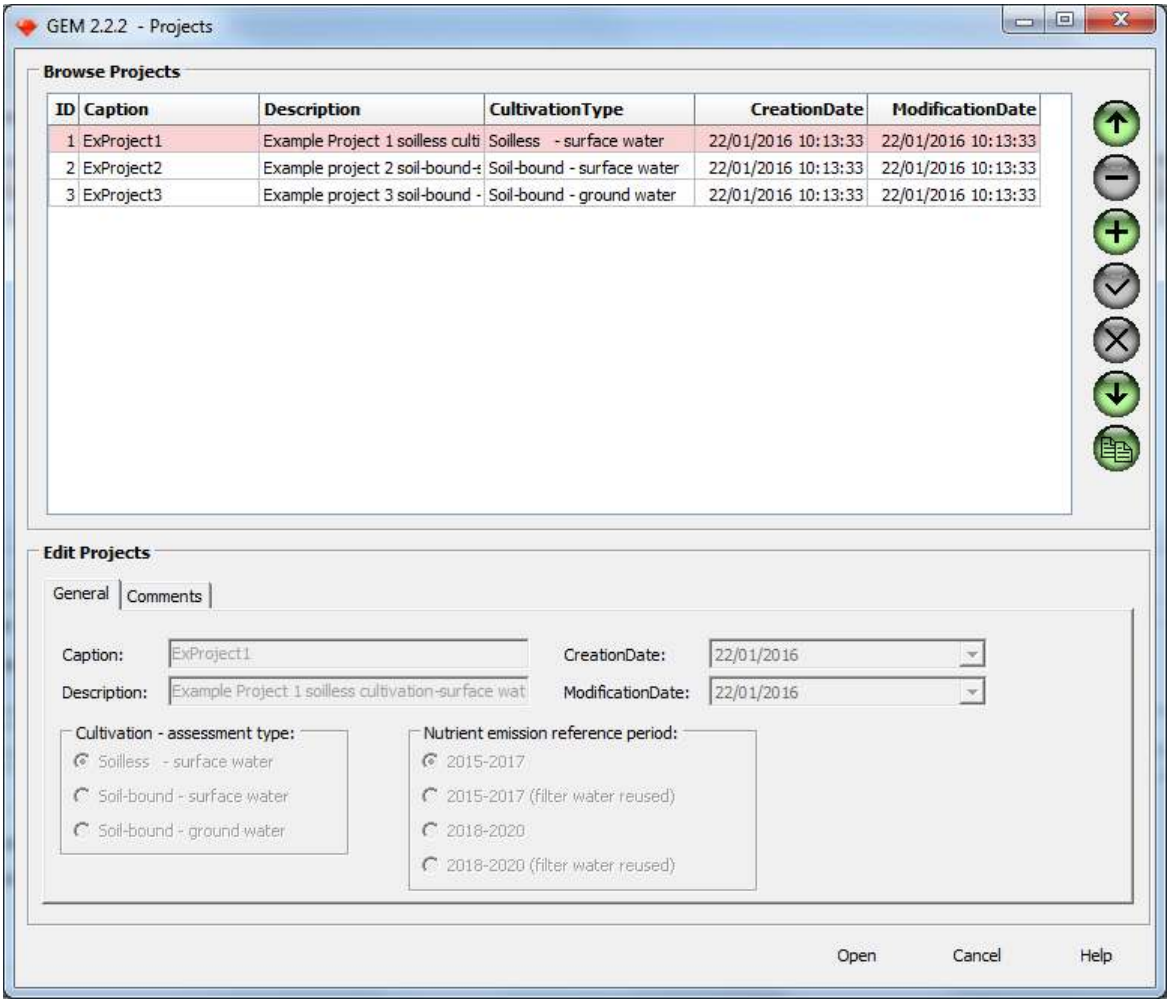
2016.02.16 Mechteld ter Horst

In this document, it is assumed that the GEM and SPIN software tools are already installed on the PCs.

- **Start GEM 2.2.2. by double clicking the GEM short cut on your desktop or in the start menu**


GEM 2.2.2

- **The GEM 2.2.2 – Project screen is opened:**

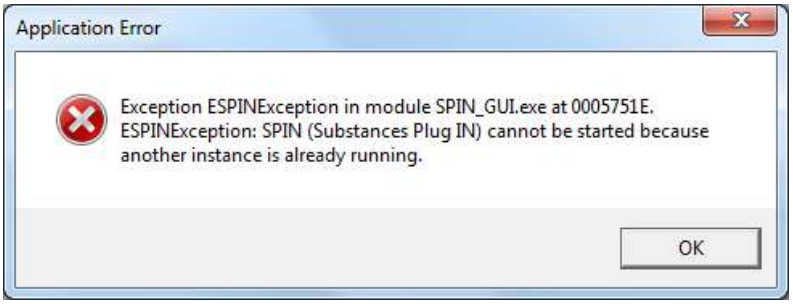


- GEM 2.2.2. contains three example projects which are locked

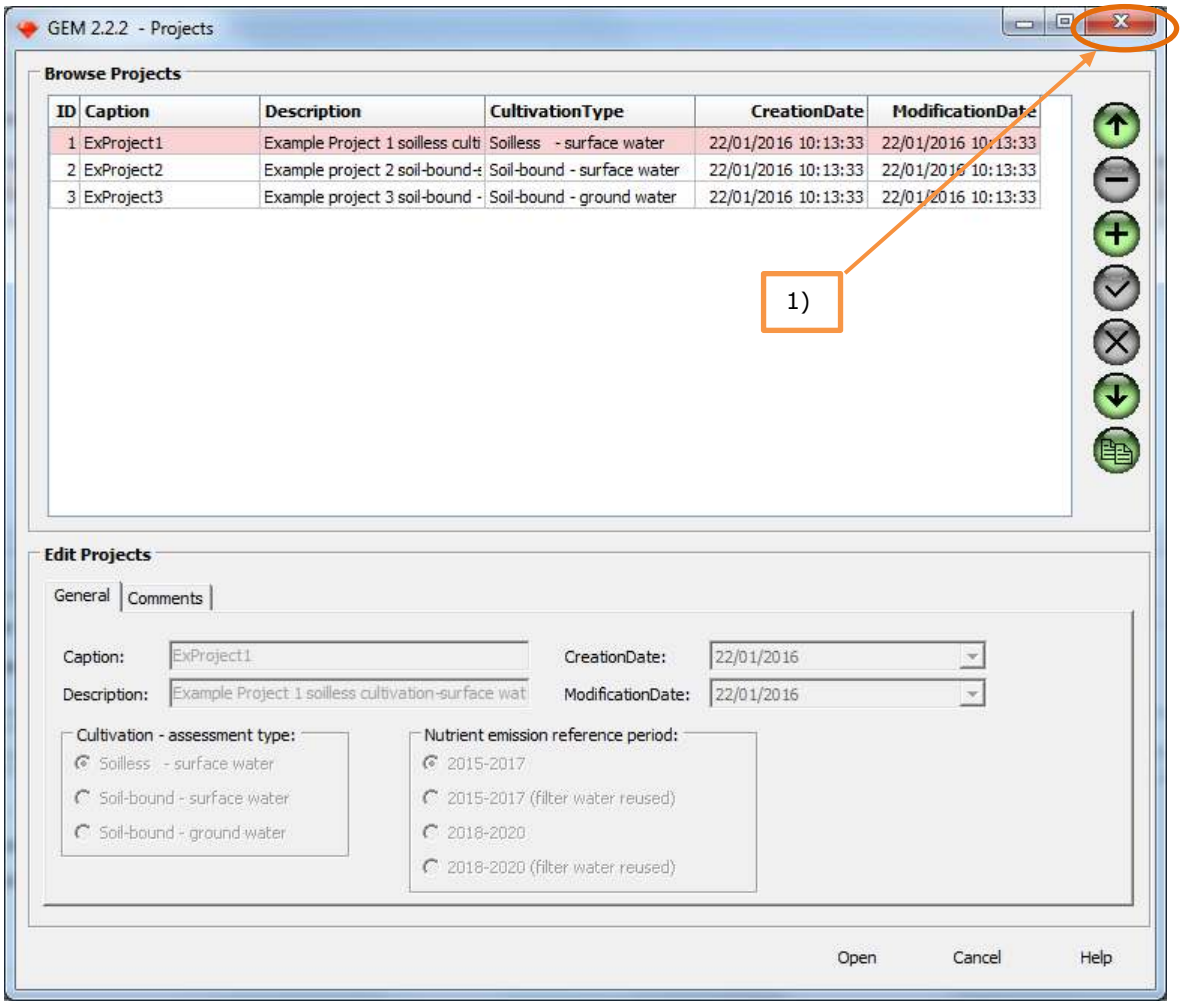
CASE 1: creating projects for soil-bound groundwater and soil-bound surface water. Proceeding with soil-bound groundwater supplying it with 1 assessment with substance Pa1T1 and 1 metabolite M1T1 (opening SPIN stand-alone) and the application scheme of CASE 1 (see Annex 1 for data)

We will start with adding substance Pa1T1 to the SPIN database. For this particular case we will use SPIN stand-alone (not via host application GEM). Note that SPIN cannot be used stand-alone if a host application is opened.

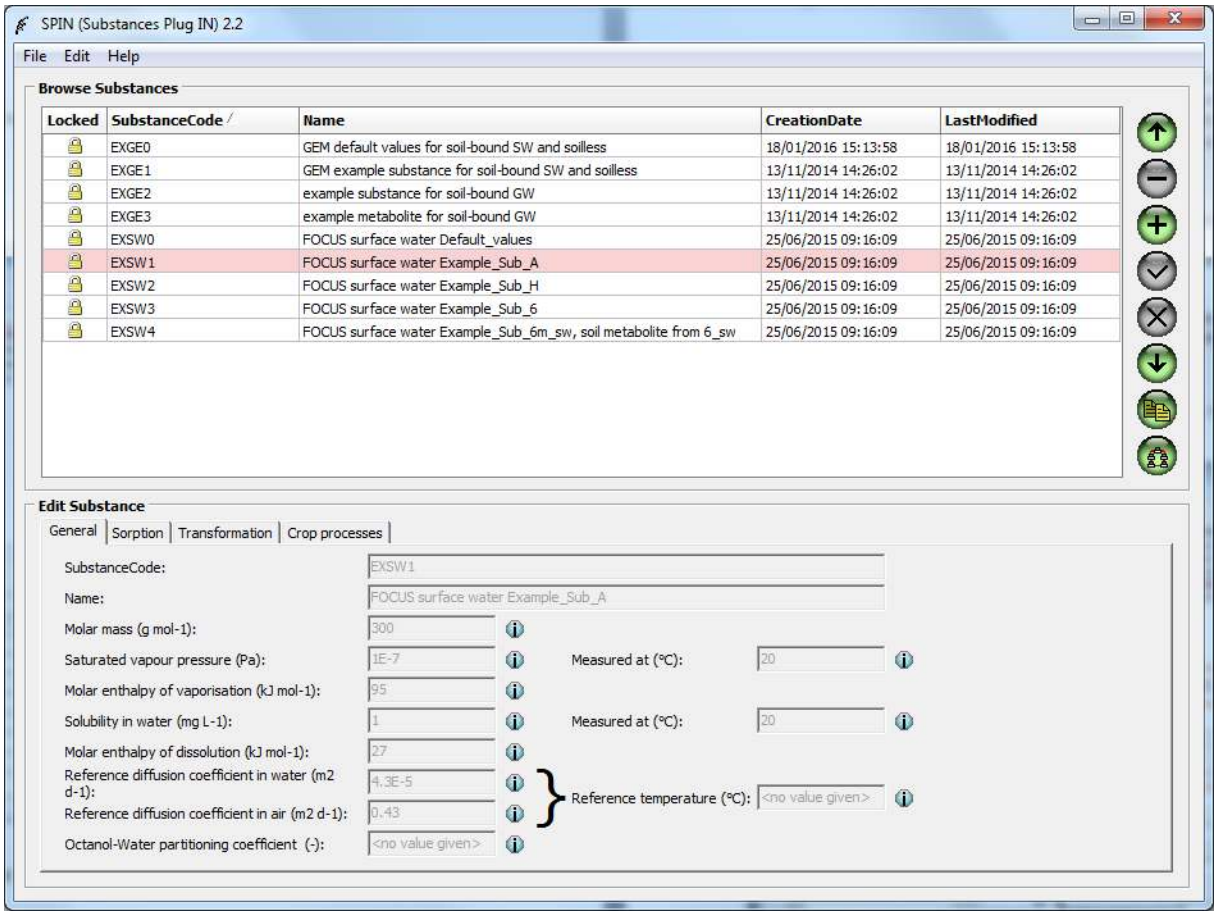
The first step is to close GEM. If this is not done and it is tried to open SPIN stand-alone the following error message will appear:



1) Close the GEM application by either clicking the red button with the white cross in the upper right corner of the Project screen of GEM.



2) Open SPIN stand-alone by clicking the SPIN icon on the desktop or in the start-menu



Several buttons exist on the right hand side of the Browse substances table; they are explained below:

 go to the first substance in the browse substances table

 delete the substance selected in the browse substances table

 define a new substance

 save the changes made by the user

 cancel the changes made by the user

 go to the last substance in the browse substances table

 copy the selected substance

 open the metabolite form

When using the '+' button to add a new substance, fields of **all** substance properties are empty. This means that default values of some substance properties are not filled in as well. Therefore, the substance

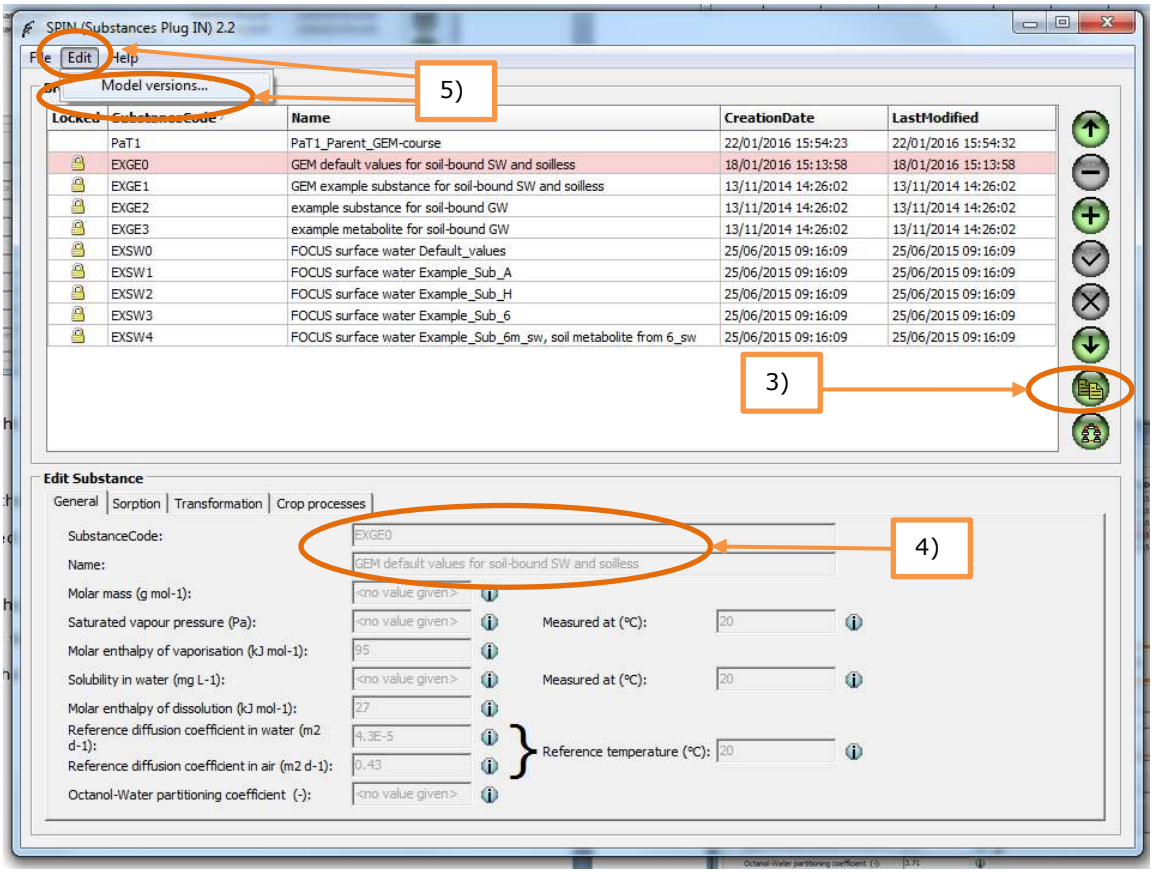
EXGE0 has been defined using current default values for activation energies, reference conditions, etc. We recommend copying this substance and edit the copied values to define the substances for the case studies.

3) Select substance EXGE0 in the Browse substances table and click the copy button: 

4) Fill in Substance code: Pa1T1 and Substance name: Pa1T1_Parent_GEM-course

Fields for all substance properties are now open for editing. The number of fields open for editing can be limited by specifying for which model versions the substance should be applicable (see 5). SPIN uses this information to check whether the minimally required information for running the models is available.

5) Click in the Menu bar on 'Edit', followed by clicking on 'Model versions...'

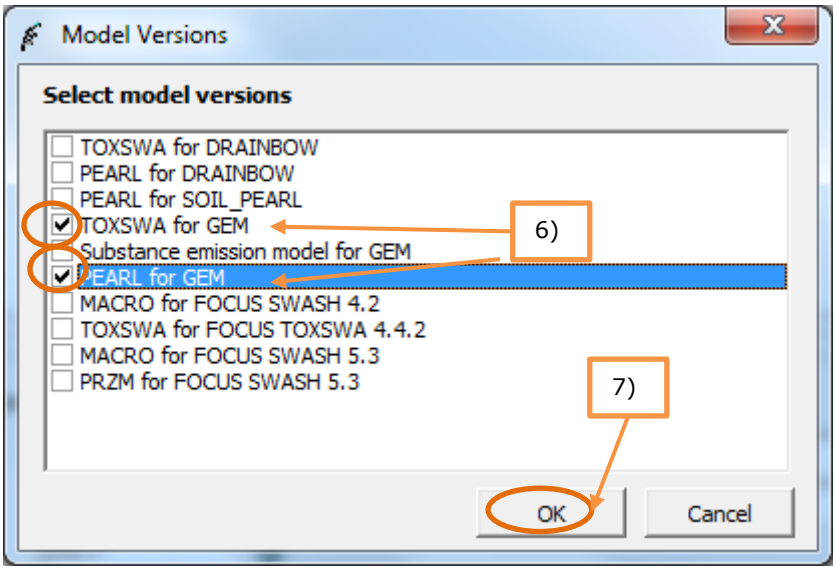


For Soil-bound groundwater water exposure assessments the model PEARL is used. For Soil-bound surface water exposure assessments the models PEARL and TOXSWA are used.

6) Select from the screen Model Version, the options 'TOXSWA for GEM' and 'PEARL for GEM' by selecting the corresponding tick boxes.

7) Click the button 'OK' to save the selected options and to close the screen Model Version

Note: check the tab transformation, subtab other – all fields are grey and locked for editing, indicating that substance property input for soilless assessments in GEM are not required.



8) Fill in all substance properties of Pa1T1 as given in Annex 1. The DegT50 of a substance in soil is measured for field soils. Multiply the DegT50 of a substance in soil with the assessment factor of 10 for first tier calculations as proposed in the soil-bound scenario report.

In the next steps you will create a metabolite forming in soil and you will link this metabolite to parent substance Pa1T1.

To link a metabolite to a parent substance, first the metabolite substance has to be created. This is done by copying EXGE0 and changing the Substance Code and Name. Also multiply the DegT50 in soil of this metabolite with the assessment factor of 10.

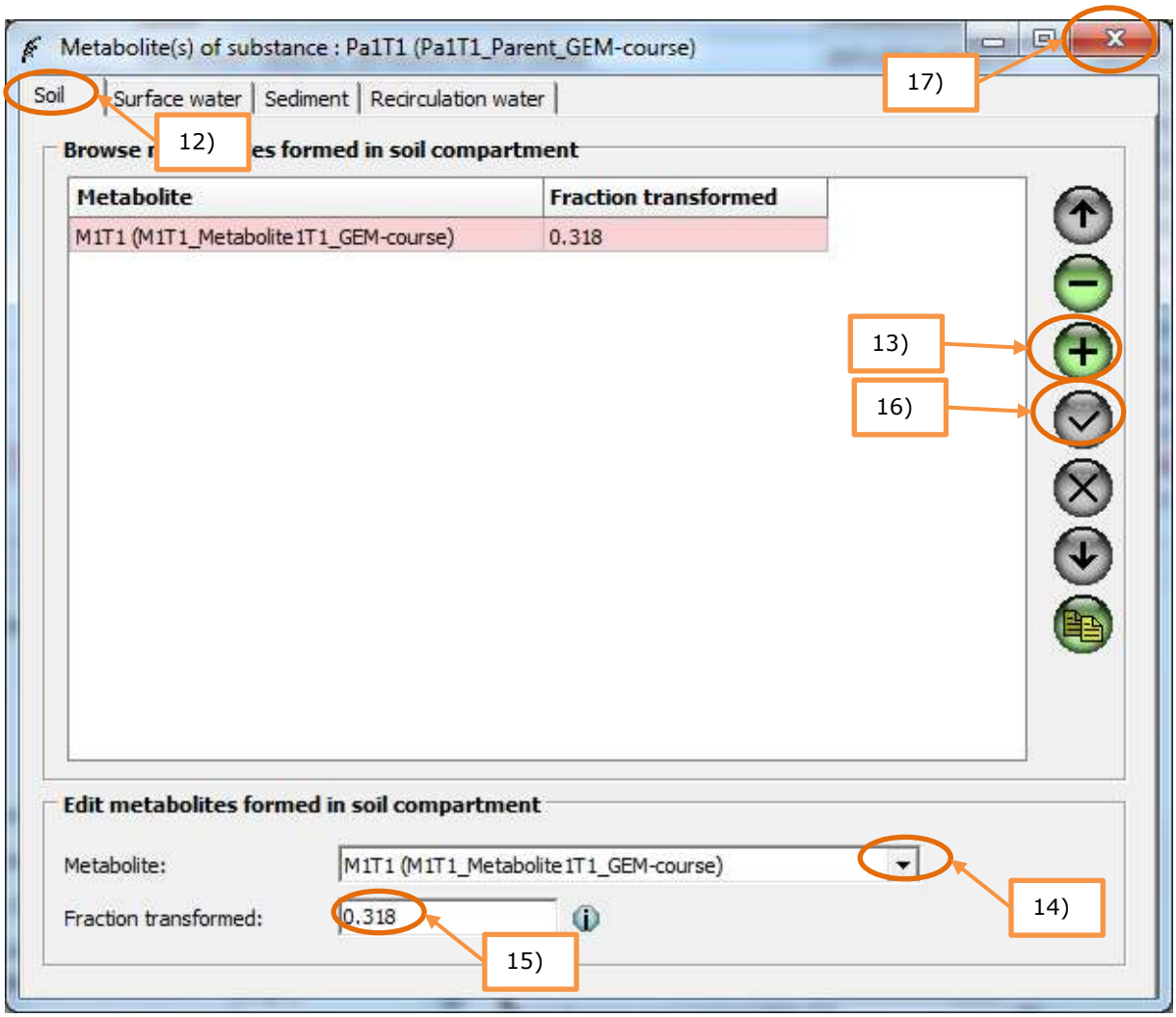
9) Select substance EXGE0 in the Browse substances table and click the copy button: 

10) Fill in Substance code: **M1T1** and Substance name: **M1T1-Metabolite1T1_GEM-course** and the substance properties for this metabolite given in Annex 1. Note to multiply the DegT50 in soil with the assessment factor of 10.

11) Select substance **Pa1T1** in the Browse substances table and click the metabolite scheme button: 

The metabolite screen shows four tabs: Soil, Surface water, Sediment and Recirculation water. These tabs represent the different compartments where the metabolite(s) can be formed. Each tab shows two parts:

- the **Browse metabolites** part. Here, all metabolites associated with a parent substance are shown.
- the **Edit metabolites** part. A metabolite can be selected from a drop-down menu and the fraction transformed can be entered.



12) Select the Soil tab in the Metabolite screen

13) Click the '+' button. Note that the fields in the **Edit metabolites** part change from grey to white colour.

14) Select M1T1 from the pick list at the right hand site of field Metabolite

15) Fill in the fraction transformed (see Annex 1) in the field of Fraction transformed

16) Save the information for M1T1 in soil by clicking the '√' button

17) Close the Metabolite screen by clicking the red button with the white cross in the upper right corner

18) Close the SPIN application by clicking the red button with the white cross in the upper right corner of the main screen of SPIN.

- **Start GEM 2.2.2 by double clicking the GEM short cut on your desktop or in the start menu**

 GEM 2.2.2

- **The GEM 2.2.2 – Project screen is opened:**

I. Projects screen

19) Click on the '+' button in the project screen to add a new project

20) Select the radio button for Cultivation – assessment type: Soil-bound – surface water

21) Type in the field for 'Caption': Case1-SBSW (Description is optional)

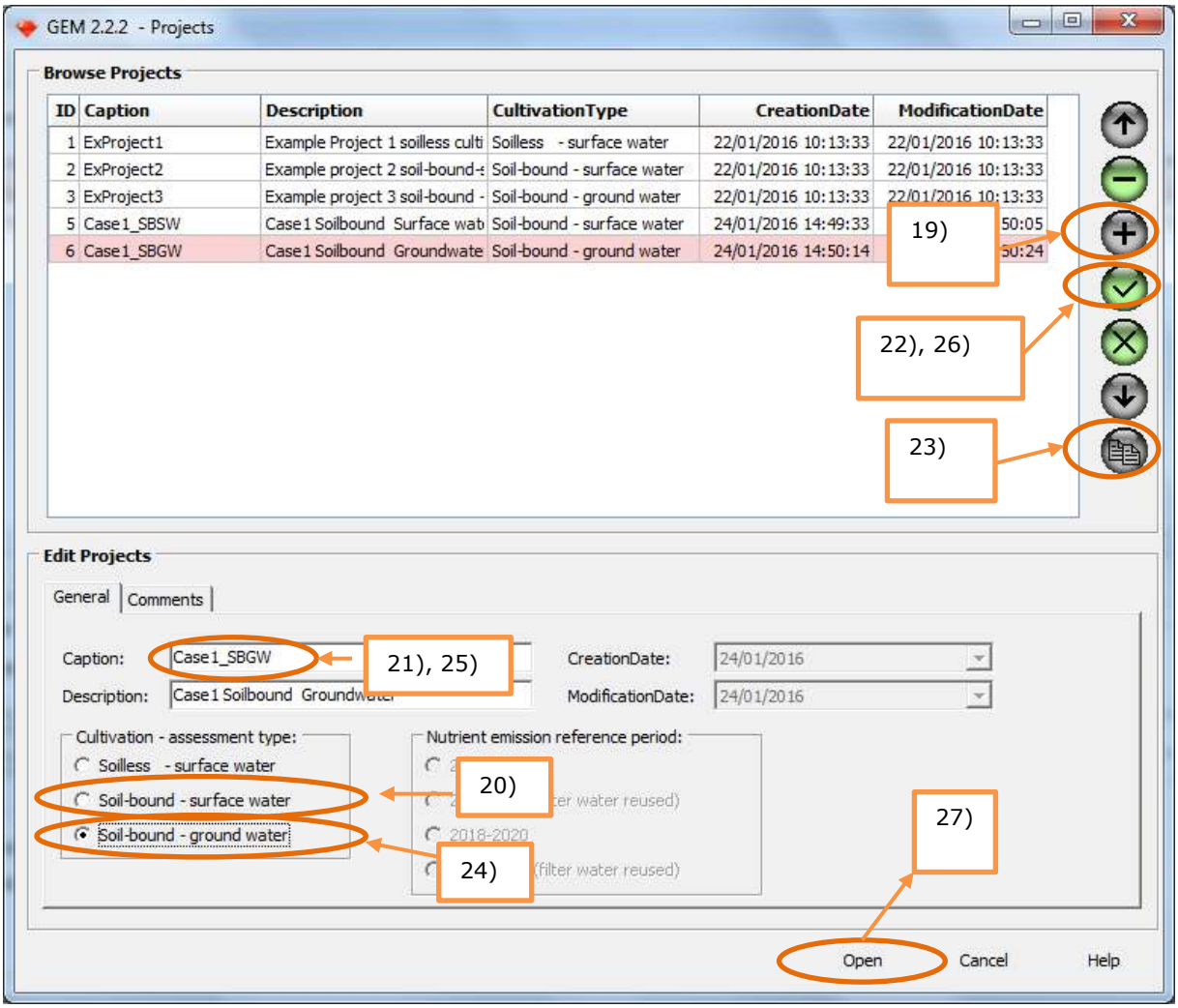
22) Save the project by clicking the '√' button

23) Select Case1-SBSW in the Browse Projects table and click on the copy  button in the project screen.

24) Select the radio button for Cultivation – assessment type: Soil-bound – ground water

25) Type in the field for 'Caption': Case1-SBGW (Description is optional)

26) Save the project by clicking the '√' button



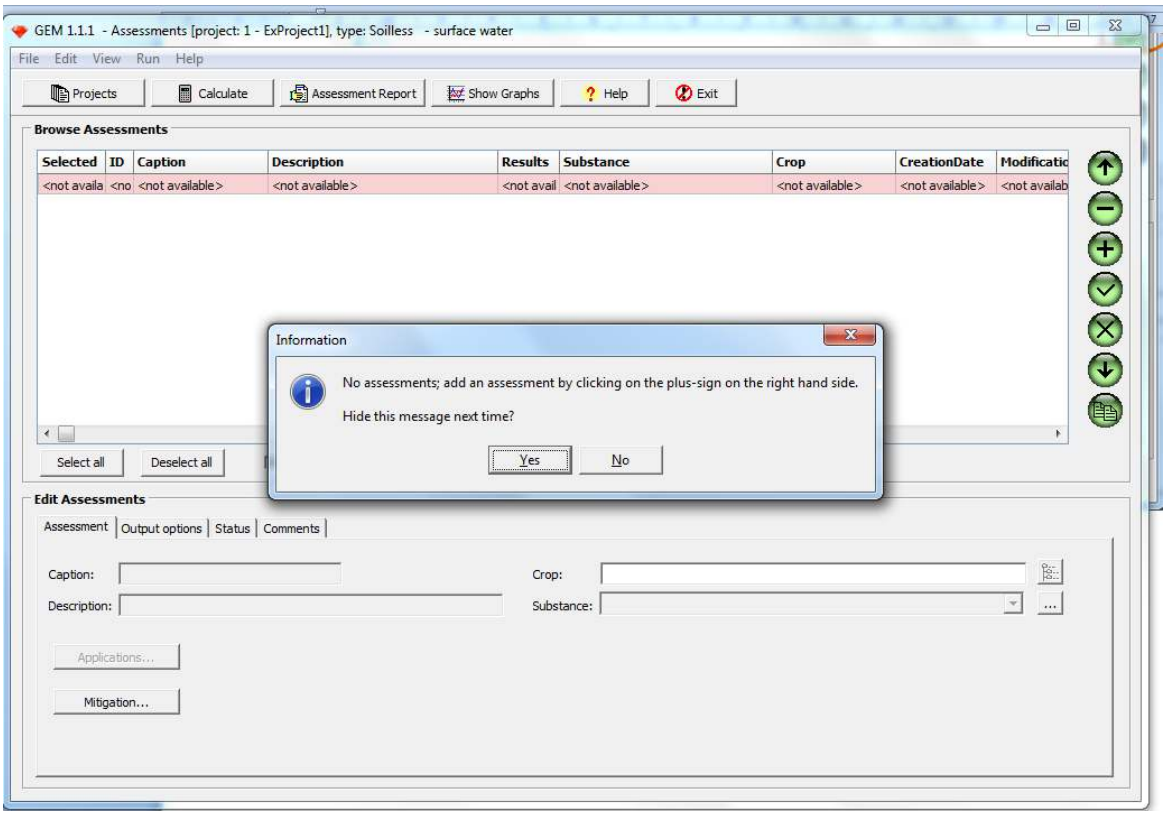
Note that after copying Case1-SBSW it is still possible to change the cultivation-assessment type, because this project does not contain any assessments yet. Once a project contains one or more assessments, the project can be copied, but the cultivation-assessment type cannot be changed anymore. You can test this later on once you filled in an assessment for Project Case1_SBGW by copying project Case1_SBGW (and deleting the copy again after checking that the cultivation-assessment type cannot be changed).

We will now proceed with the soil-bound groundwater project Case1-SBGW.

27) Click the 'Open' button to open the Project: Case1-SBGW

Assessments screen

28) A hint is given for the next step (how to add an assessment): Click 'Yes'



29) Click on the '+' button in the Assessments screen to add a new assessment

The new assessment will receive an ID number in consecutive order.

- ExProject1 -> assessment IDs: 1, 2
- ExProject2 -> assessment ID: 3
- ExProject3 -> assessment ID: 4
- Case1_SBGW -> assessment ID: 5

In the section 'Edit Assessments' the tab 'Assessment' is shown by default.

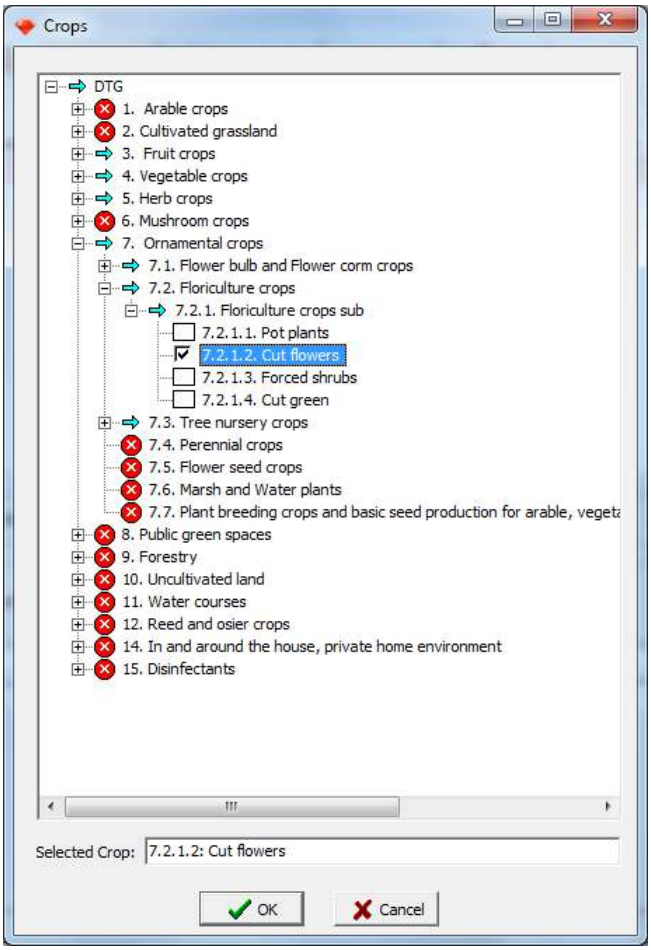
Caption/Description

30) Type in the field for 'Caption': 'Case1_SB_GW_A1' (Description is optional)

Crop

31) Select the crop: '7.2.1.2 Cut flowers' from the DTG list. Clicking on the button at the right hand site of the field for 'Crop' will open the 'Crops' screen containing the DTG list.

The 'Crops' screen is opened (see Annex 3 for more information on how to use this screen). By clicking the small boxes with the + symbol the DTG list is expanded.

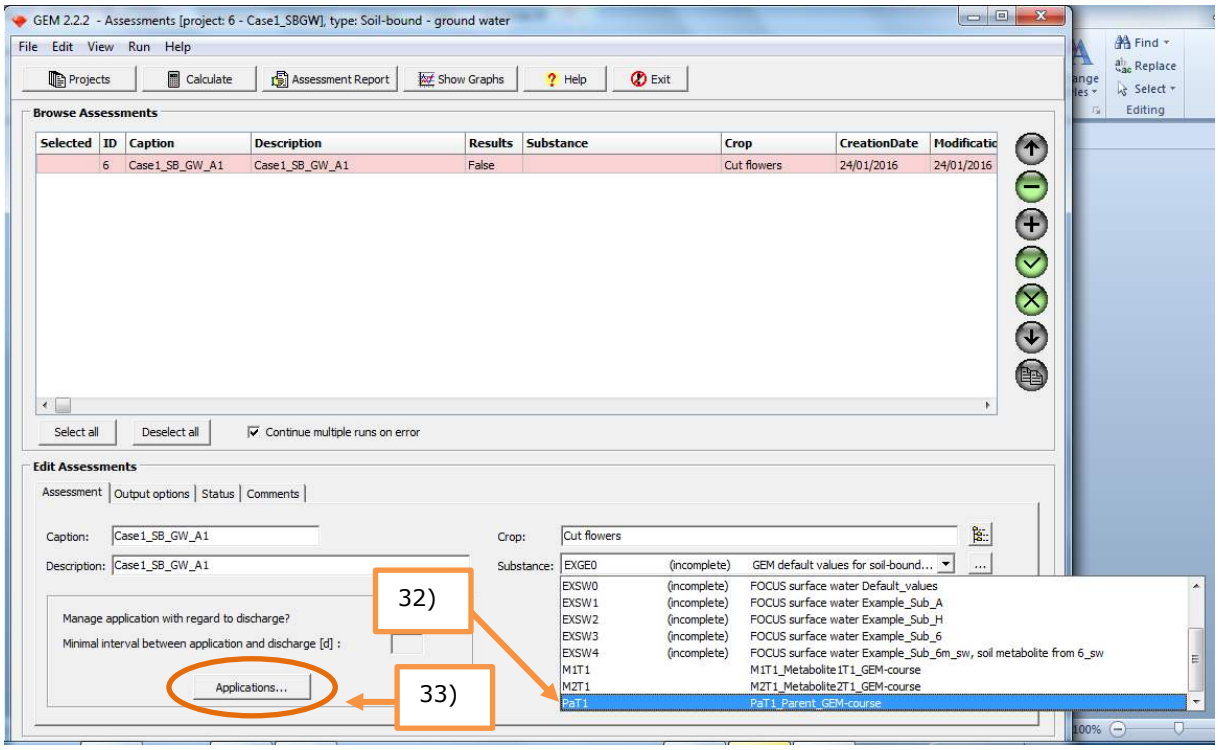


Note that for soil-bound the crop is more or less a dummy, because all soil-bound groundwater and surface exposure assessments in GEM the crop parameters in PEARL use the values of the crop CHRYSANT (see GEM Manual, Section 1.3)

Substance

32) Select substance Pa1T1 from the picklist by clicking the box with the arrow on the right hand site of the field Substance.

33) Click the button 'Applications'



The GEM 2.2.2 Applications screen appears

34) Click the '+' button to add a new application event

The application data for 'Case1_SB_GW_A1' are found in Annex 1

35) Select the application type from the picklist by clicking the box with the arrow at the right hand site of the field Application Type.

36) Select the month and day of the application from the picklists by clicking the boxes with the arrow at the right hand site of the field Application Date.

37) Fill in the dosage in the field of Dosage

38) Set the Fraction intercepted (to 0.5 in this example)

39) Save the application by clicking the '√' button

Steps 34 – 39 need to be repeated for each application. It is usually quicker to use the 'copy' option for adding applications.

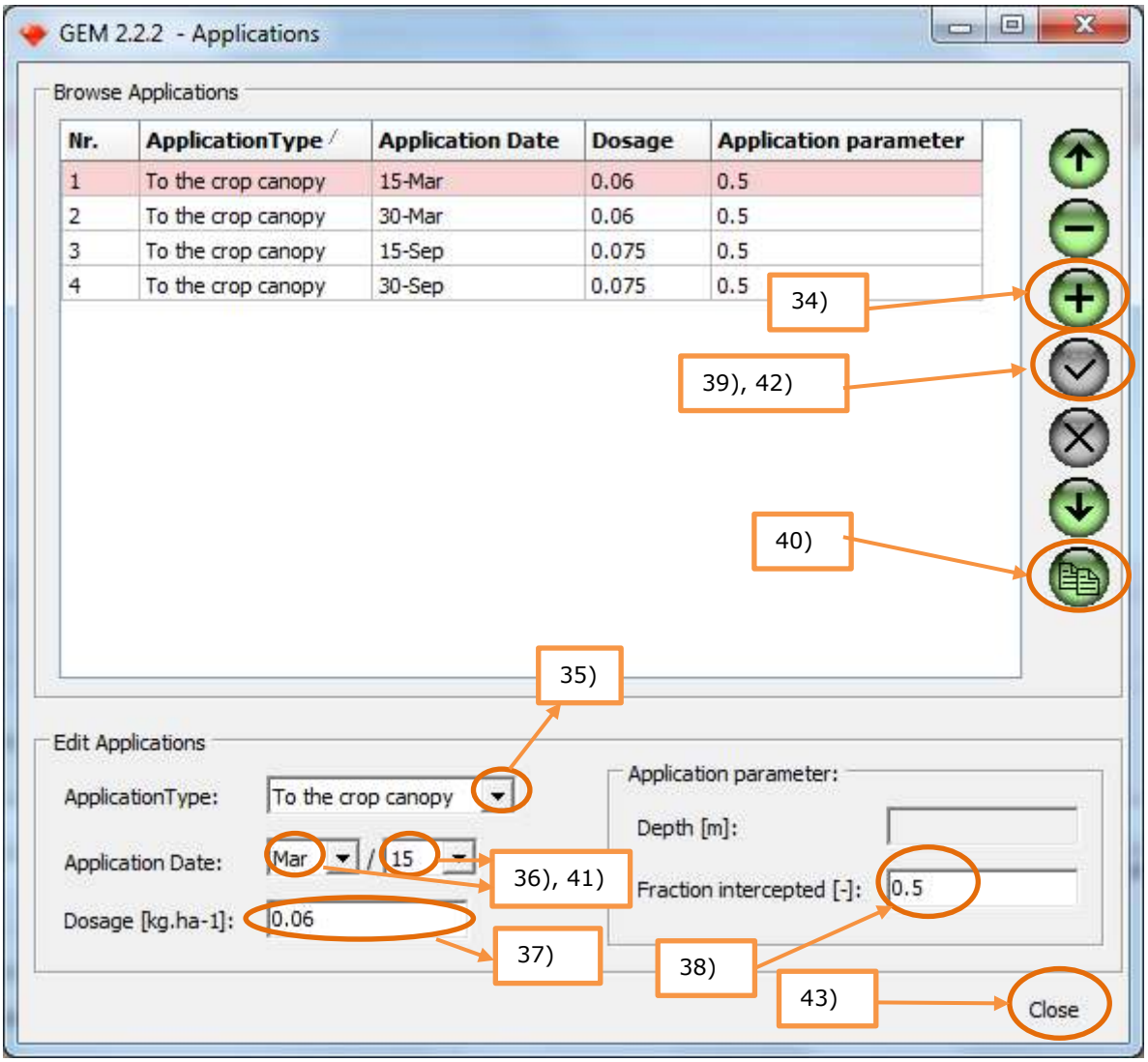
40) For adding the second application click on the button:  (copy)

Note that the date of the copy of the application is automatically set to the following day.

41) Change the day of application: select the appropriate day from the picklists by clicking the box with the arrow at the right hand site of the field Application Date

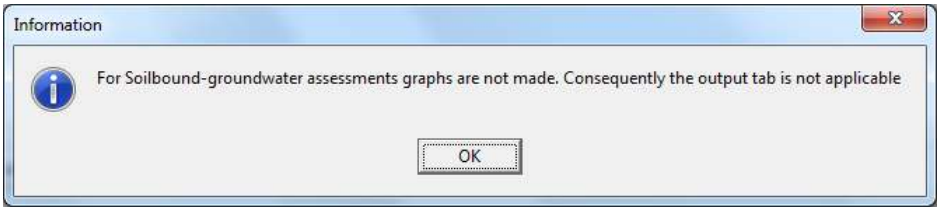
42) Save the application by clicking the '√' button

43) Leave the Application screen by clicking the 'Close' button



Note the Mitigation button on the Assessments screen is disabled for Soil-bound projects/assessments

For Soil-bound **Groundwater** exposure assessments it is not necessary to fill in or change properties on the output tab. If trying so, the following message will be shown:



At this moment all information needed for the simulation is entered into the software tools. The next step is to prepare the assessment(s) for simulation.

Three steps are necessary here:

1. Select the assessment(s) for simulation
2. Decide on whether to enable or disable 'Continue multiple runs on error'
3. Start the simulation(s)

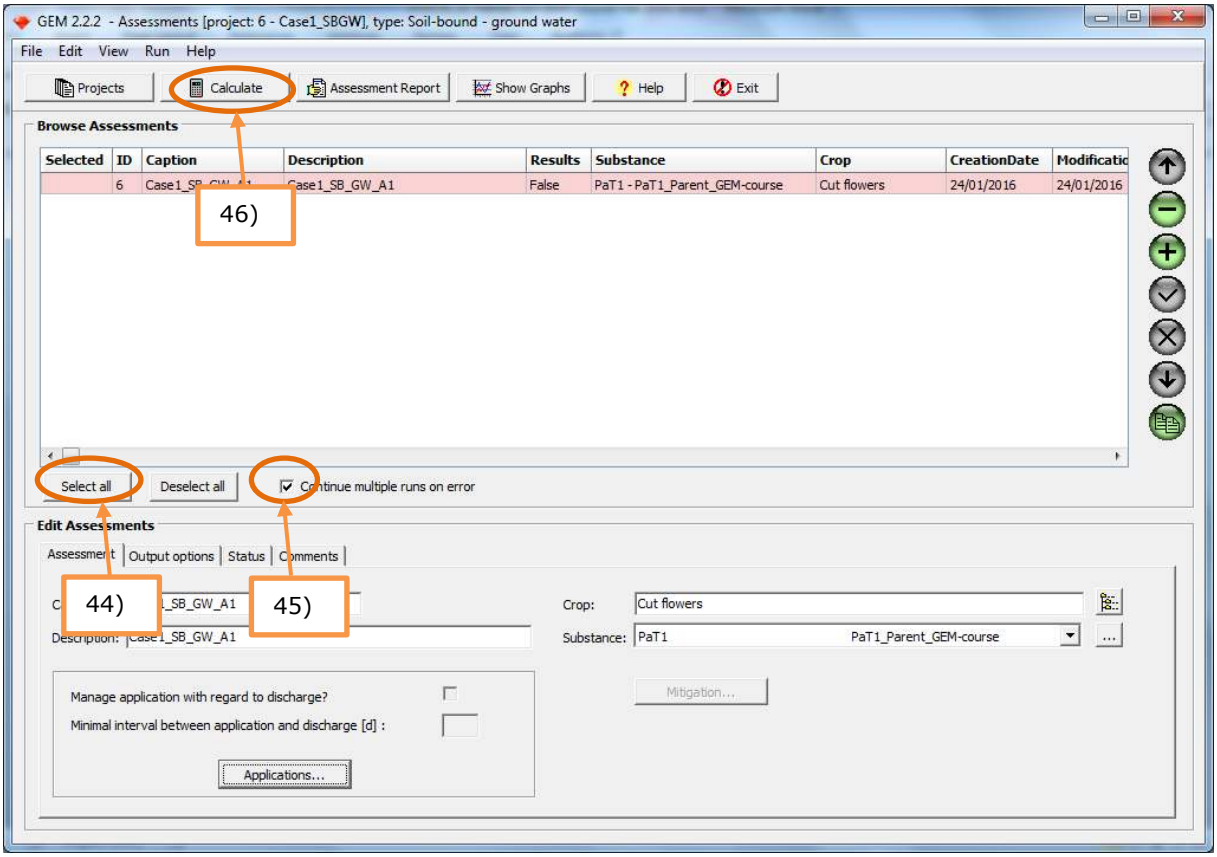
44) Click the button 'Select all'. Note that the column 'Selected' in the Browse Assessments table is filled with 'Yes' indicating that the assessment is selected for simulation.

45) Disable 'Continue multiple runs on error' ; the tick box should be empty (in case of errors a notification will be given via a pop-up message)

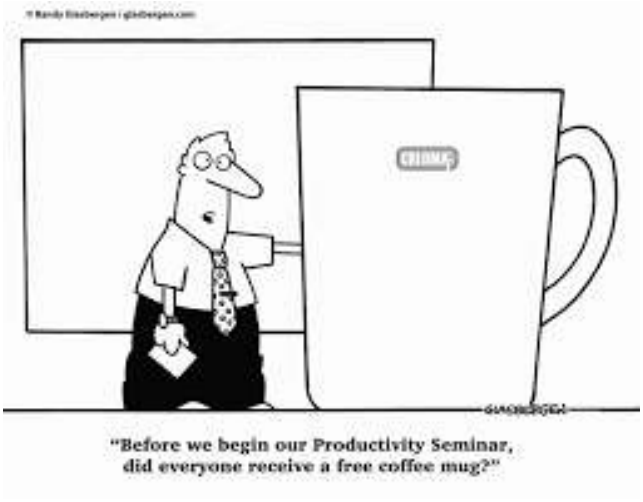
Continue multiple runs on error: This option is enabled by default (wish of the Ctgb). It allows the program to continue its calculations with the next assessment in case of a failed assessment. Setting the option to the 'enabled' state allows the calculations to continue without an error message being 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 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

46) Click the button 'Calculate'



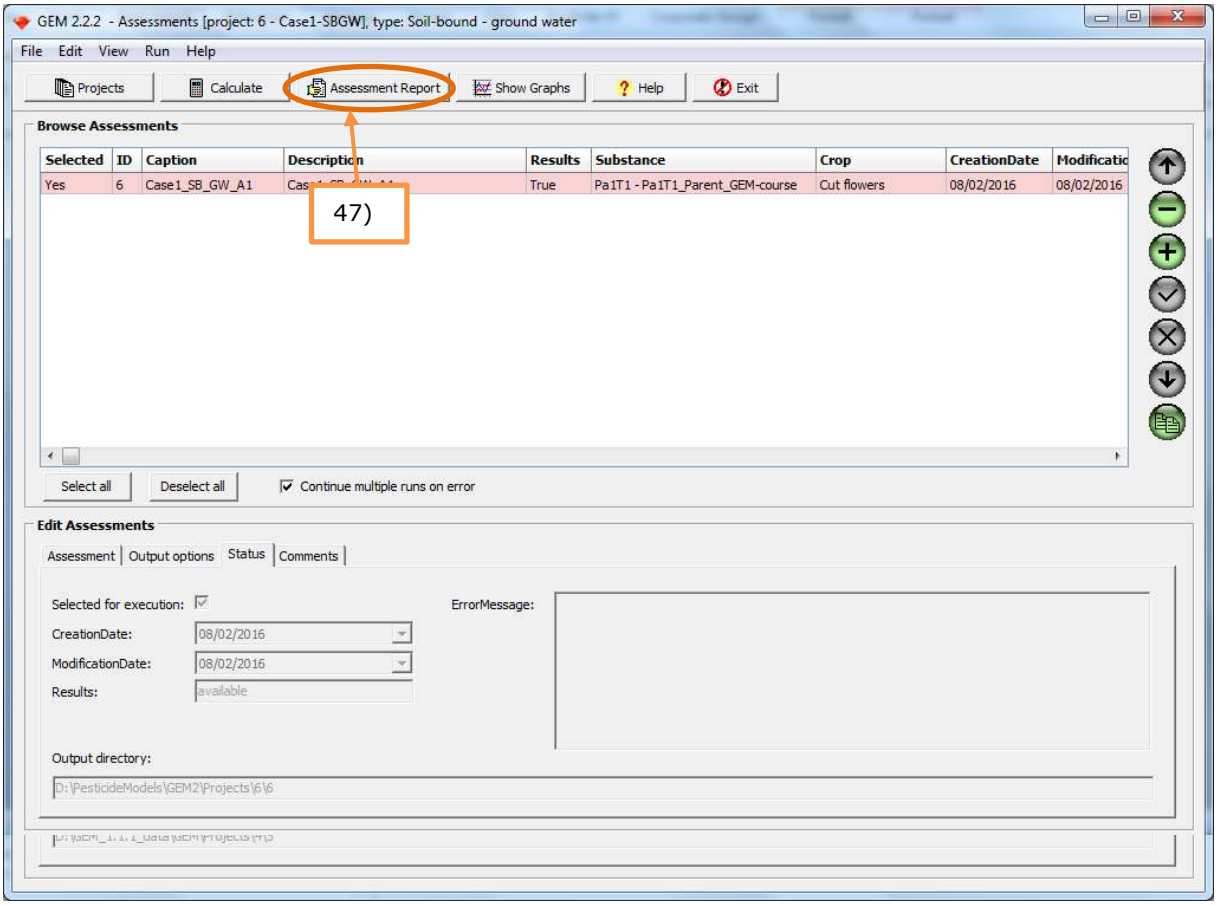
Two models need to be run in consecutive order to calculate the groundwater leaching concentration. The SWAP model calculates the hydrology in the greenhouse soil, PEARL simulates the PPP fate in the greenhouse soil and calculates the groundwater concentrations as well as the end point concentration. The models are run over the period 1981 to 2007, with a warming up period of six years. This will take about 5-10 minutes, so time to take some tea/coffee.



After the break, proceed with viewing the results of the simulation of CASE 1 Soil-bound – Groundwater

Viewing results of the simulation of CASE 1 Soil-bound – Groundwater

On the tab Status you can check whether the run did finish without errors. In case of an error the error message is displayed in the field ErrorMessage.



47) To open the assessment report click on the button 'Assessment Report'. The report (htm file) is automatically opened in the web browser of your pc.

Open the assessment report and read out the 90th percentile concentration for both the parent and the metabolite.

90th percentile PEC groundwater Pa1T1----------

90th percentile PEC groundwater M1T1----------

Would the substance be approved (groundwater water criterion = 0.1 µg/L and criterion for groundwater water abstraction areas = 0.01 µg/L)?

Suppose if not, what could the applicant do in a higher tier to decrease the Predicted Environmental Concentration?

The results of the simulation of CASE 1 Soil-bound – Groundwater will be discussed later on this afternoon. Please proceed now with the soil-bound-surface water project of CASE 1.

CASE 1: Adding an assessment to the for soil-bound-surface water project: 1 assessment with substance Pa1T1 (incl. metabolite M1T1)

48) If you are still working in the assessments screen of Project Case1_SBGW, then click the Projects button to go back to the Projects screen

49) In the Projects screen, select Project Case1_SB_SW and then click the button 'Open'.

50) Click on the '+' button in the Assessments screen to add a new assessment

The new assessment will receive an ID number in consecutive order.

- ExProject1 -> assessment IDs: 1, 2
- ExProject2 -> assessment ID: 3
- ExProject3 -> assessment ID: 4
- Case1_SBGW -> assessment ID: 5
- Case1_SBSW -> assessment ID: 6

In the section 'Edit Assessments' the tab 'Assessment' is selected by default.

Caption/Description

51) Type in the field for 'Caption': 'Case1_SB_SW_A1' (Description is optional)

Crop

52) Select the crop: '7.2.1.2 Cut flowers' from the DTG list. Clicking on the button at the right hand site of the field for 'Crop' will open the 'Crops' screen containing the DTG list.

Note that for soil-bound the crop is more or less a dummy, because all soil-bound groundwater and surface exposure assessments in GEM the crop parameters in PEARL use the values of the crop CHRYSANT (see GEM Manual, Section 1.3)

Substance

53) Select substance Pa1T1 from the picklist by clicking the box with the arrow on the right hand site of the field Substance.

54) Click the button 'Applications'

The GEM 2.2.2 Applications screen appears

55) Click the '+' button to add a new application event

The application data for 'Case1_SB_SW_A1' are found in Annex 1

56) Select the application type from the picklist by clicking the box with the arrow at the right hand site of the field Application Type.

57) Select the month and day of the application from the picklists by clicking the boxes with the arrow at the right hand site of the field Application Date.

58) Fill in the dosage in the field of Dosage

59) Set the Fraction intercepted to 0.5

60) Save the application by clicking the '√' button

Steps 55 – 60 need to be repeated for each application. It is usually quicker to use the 'copy' option for adding applications.

61) Leave the Application screen by clicking the 'Close' button

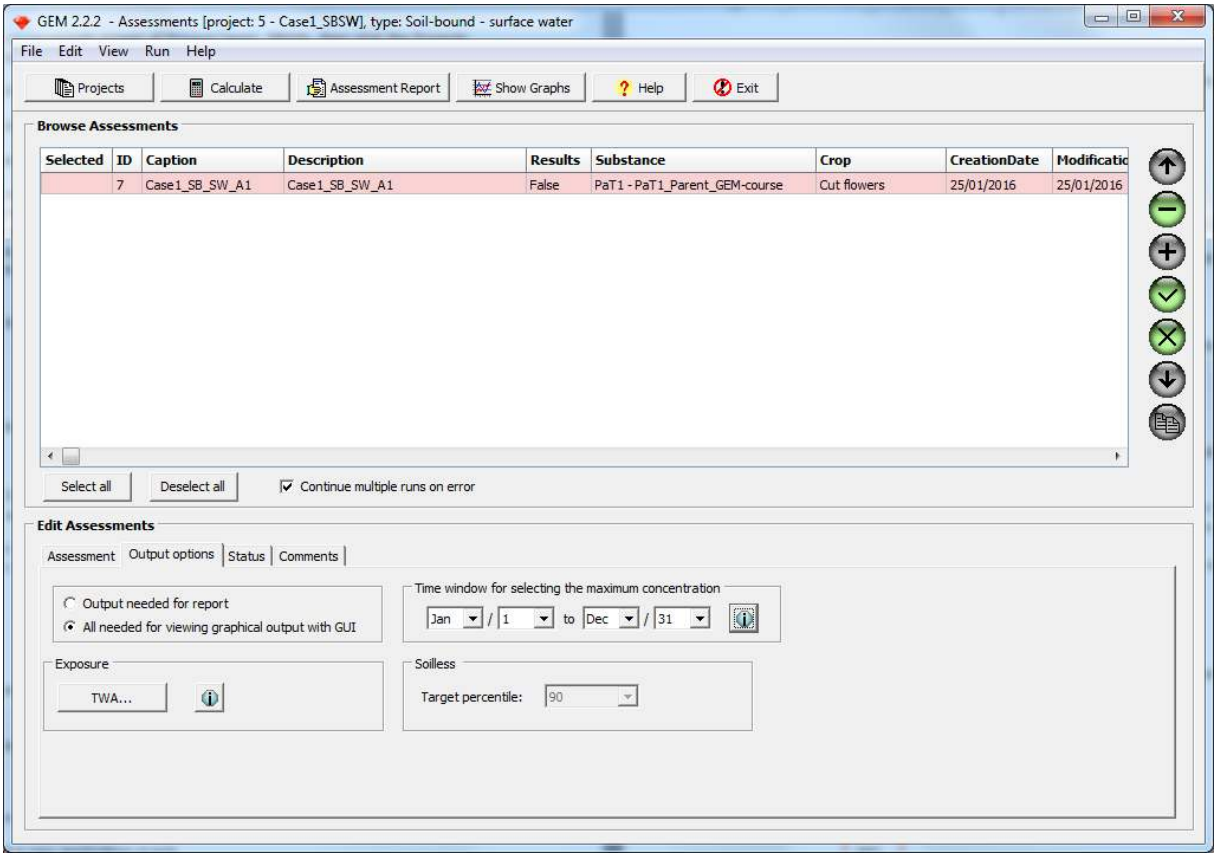
Note the Mitigation button on the Assessments screen is disabled for Soil-bound projects/assessments

For Soil-bound **Surface water** exposure assessments you have the opportunity to fill in or change properties on the output tab.

62) Go to the tab 'Output options'

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.

63) Select 'All needed for viewing graphical output with GUI



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

of 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). At this moment all information needed for simulation is entered into the software tools.

64) The time window given by default should be selected: 1 Jan – 31 Dec

TWA button: The software will by default calculate and report Time Weighted Average (TWA) concentrations calculated over periods of 7 days (TWA7d) and 21 days (TWA21d). 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. The number of TWA entries and the selected time window per entry are assessment specific properties; they have to be defined per assessment.

65) Default TWA entries (TWA7d and TWA21d) are automatically selected. You can check this by clicking the button TWA. The TWA screen will be opened. Leave it by clicking the 'Close' button on the TWA screen.

The next step is to prepare the assessment(s) for simulation.

66) Click the button 'Select all'. Note that the column 'Selected' in the Browse Assessments table is filled with 'Yes' indicating that the assessment is selected for simulation.

67) Disable 'Continue multiple runs on error' ; the tick box should be empty (in case of errors a notification will be given via a pop-up message)

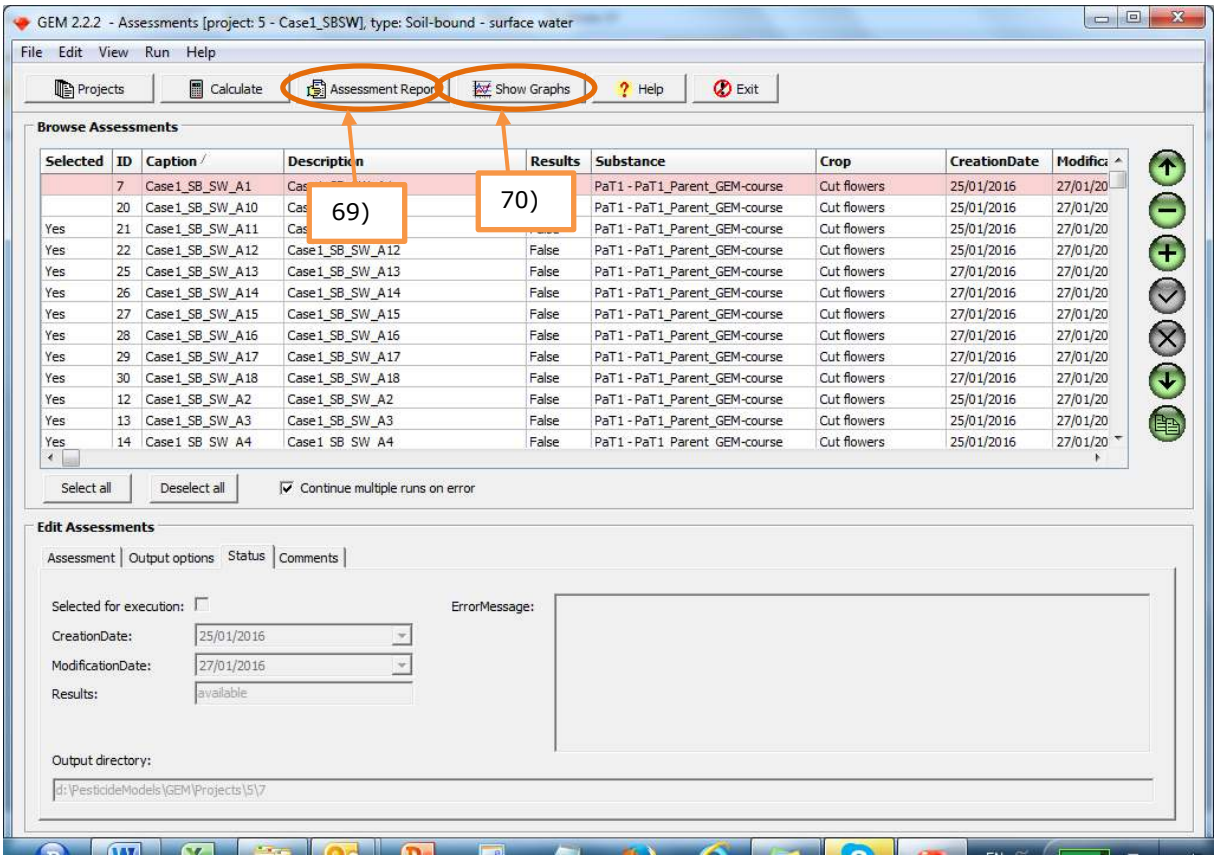
68) Click the button 'Calculate'

First the PEARL model will be run and then the TOXSWA model will be run. This will take about 60 minutes (TOXSWA needs about 30 minutes for each substance – we have two: Pa1T1 and M1T1).

The results of Case 1 will be extracted from GEM and discussed later on this afternoon.

Viewing results of the simulation of CASE 1 Soil-bound-Surface water

69) To open the assessment report click on the button 'Assessment Report'. The report (htm file) is automatically opened in the (default) web browser of your pc.



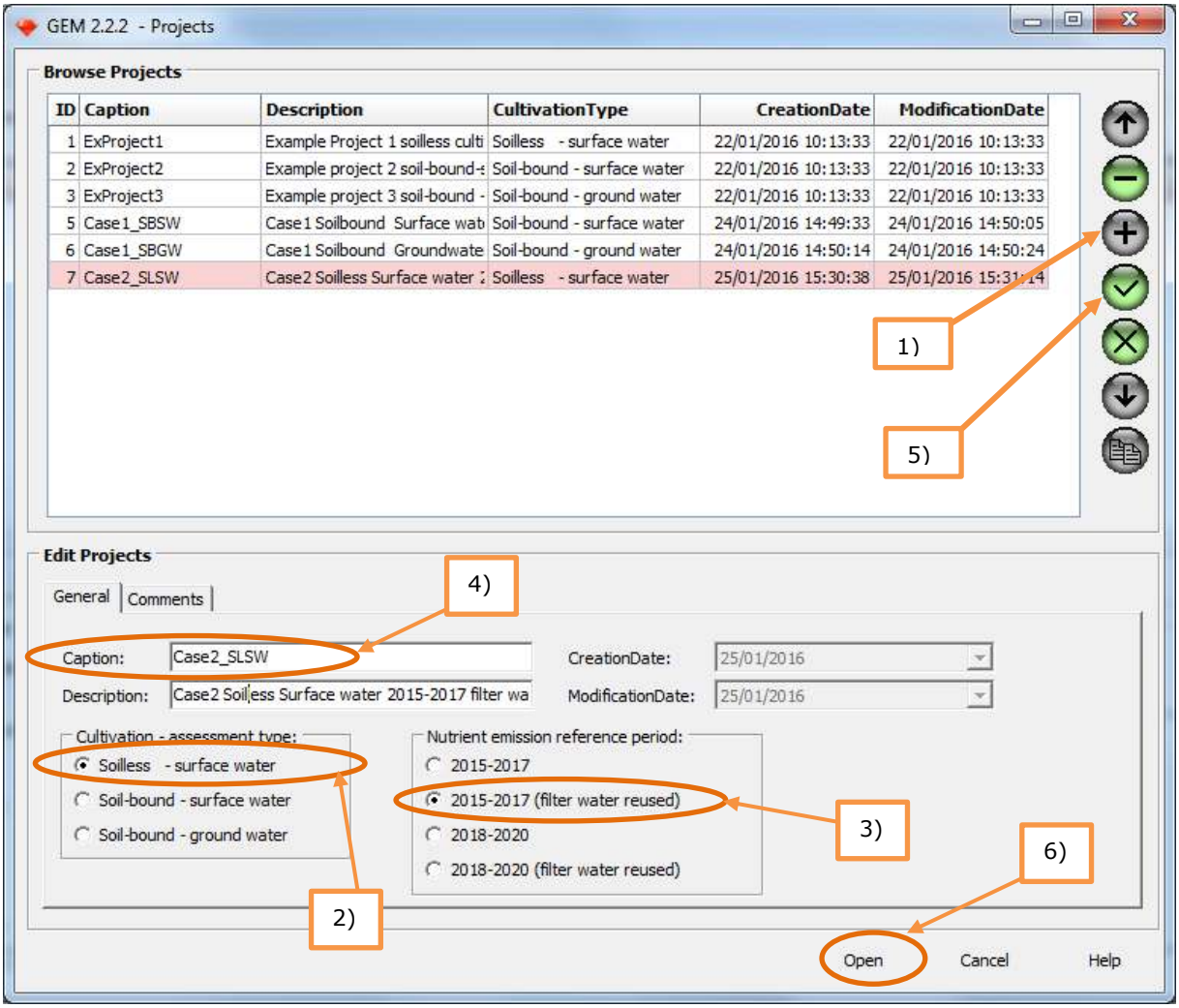
Read out the 90th percentile concentration for both the parent and the metabolite.

90th percentile PEC surface water Pa1T1----------

90th percentile PEC surface water M1T1----------

The corresponding Regulatory Acceptable Concentration for the parent substance is 1.3 µg/L (L(E)C50 invertebrates) times an assessment factor of 0.01. The corresponding Regulatory Acceptable Concentration for the metabolite is 1100 µg/L (L(E)C50 fish) times an assessment factor of 0.01. Would this substance be approved?

CASE 2: creating a project for soilless-surface water containing 1 assessment with substance Pa1T2 (opening SPIN via host GEM), an application scheme (see Annex 2 for data) and mitigation option.



I. Projects screen

1) Click on the '+' button in the project screen to add a new project

When adding a new project the user has a choice between soilless or soil-bound scenarios, where the soilless scenarios offer a further choice of the nutrient emission reference period (either 2015 – 2017, or 2018 – 2020) and the choice whether or not the calculations should presume the reuse of filter water. These choices are not presented when selecting a soil-bound scenario.

The effect of choosing either the 2015 – 2017 or the 2018 – 2020 reference period reflects the change in strictness of emission rules from 2018 onward. Emissions because of possible damage to crops due to high salt concentrations are still allowed. For the earlier period 2015 – 2017 a higher overall volume of emissions were permissible (and included in the calculations).

2) Select the radio button for Cultivation – assessment type: Soilless – surface water

3) Select the radio button for Nutrient emission reference period: 2015-2017 (filter water reused)

4) Type in the field for 'Caption': Case2_SLSW (Description is optional)

5) Save the project by clicking the '√' button

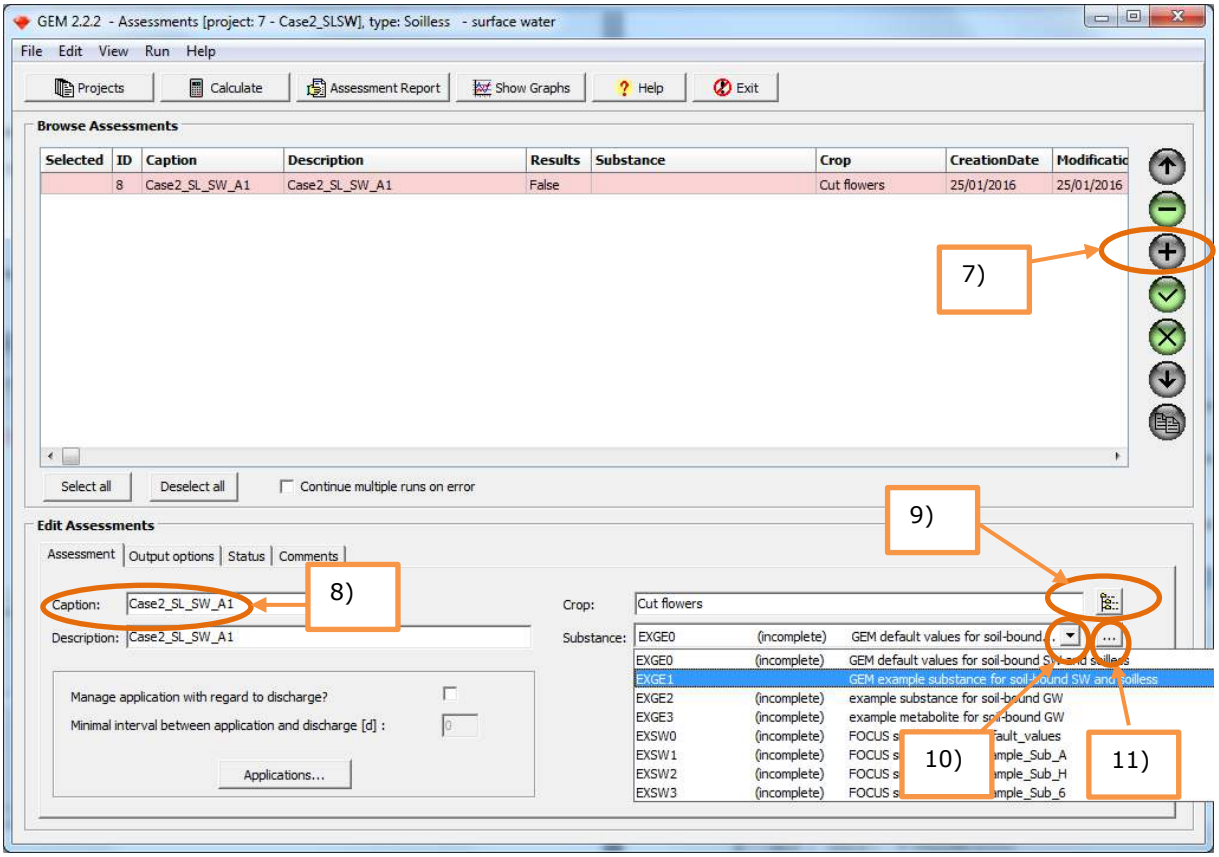
6) Click the 'Open' button to open the Project

II. Assessments screen

7) Click on the '+' button in the Assessments screen to add a new assessment

Caption/Description

8) Type in the field for 'Caption': 'Case2_SL_SW_A1' (Description is optional)

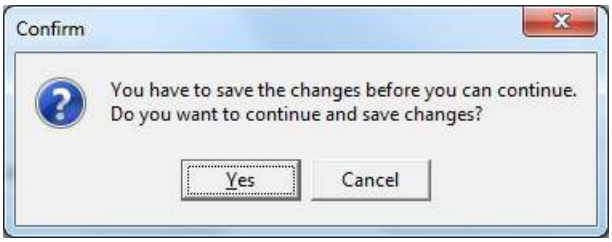


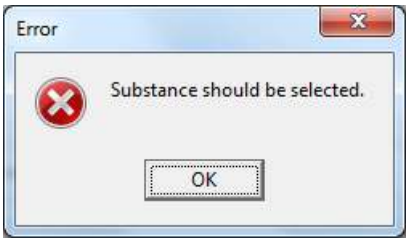
Crop

9) Select the crop: '7.2.1.2 Cut flowers' from the DTG list. Clicking on the button at the right hand site of the field for 'Crop' will open the 'Crops' screen containing the DTG list.

Substance

In GEM substances are managed via the SPIN (Substance PlugIn) tool. SPIN can be opened by clicking the  button at the right hand site of the Substance field. If doing so you will see the following two message screens in consecutive order:

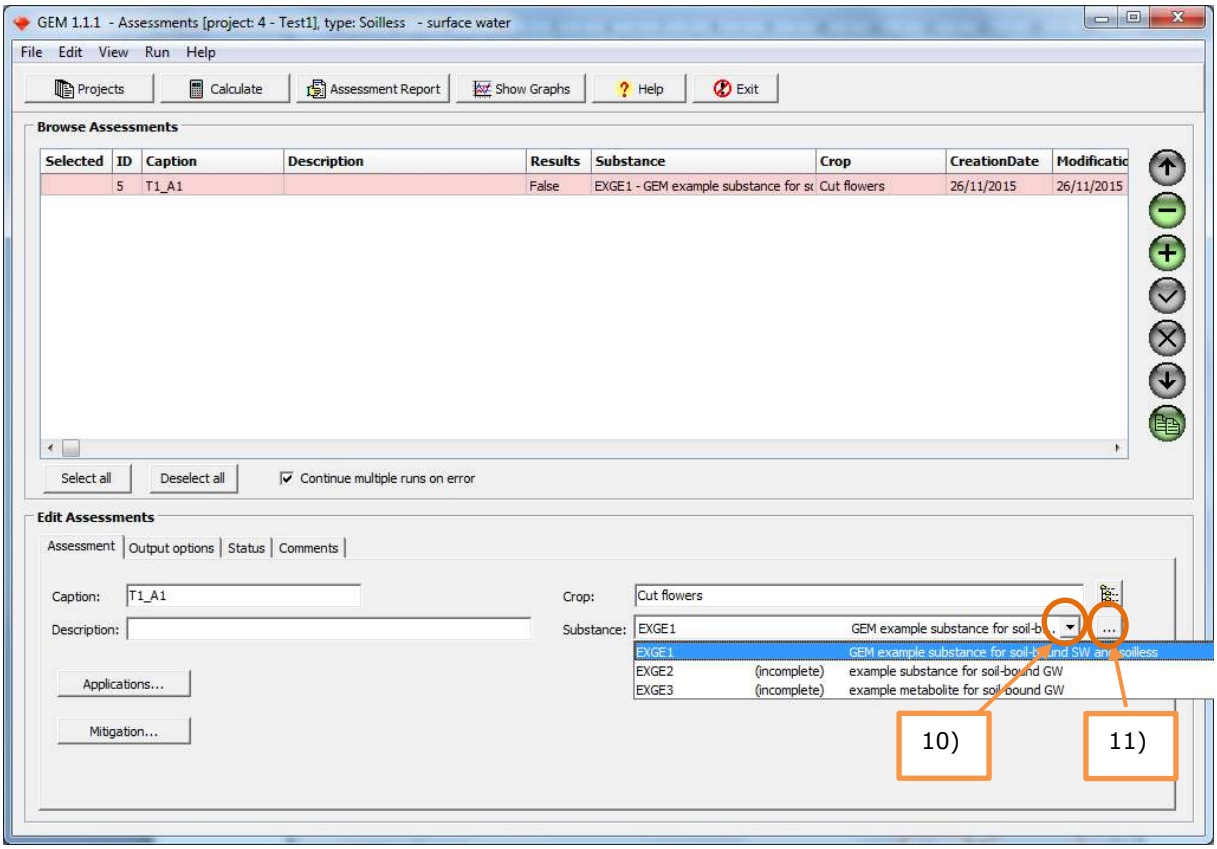




Above two messages indicate that you should first select an existing substance for the assessment before you can proceed adding a new substance to the SPIN database.

10) Select EXG1 from the picklist by clicking the box with the arrow at the right hand site of the field Substance.

11) Click the  button at the right hand site of the Substance field to open SPIN. Note again that you have to select a substance from the pick list before you can open SPIN.



SPIN

12) Copy substance EXG0 to add a new substance to the SPIN database containing all default values.

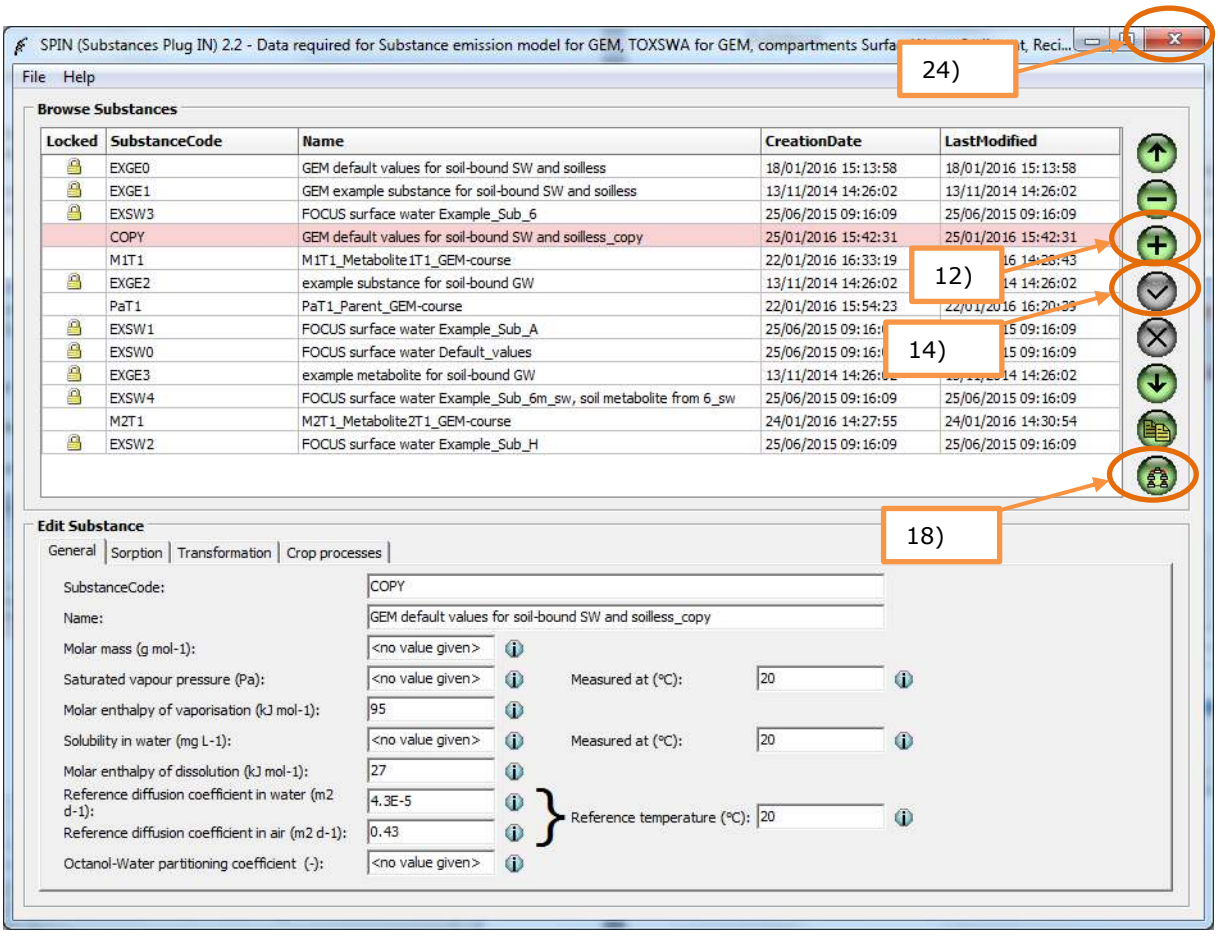
Check out the four different main tabs (General, Sorption, Transformation, Crop processes) and the different subtabs (e.g. for Sorption – subtabs: Soil, Surface water, Sediment, Substrate).

You will notice that fields which require input for this specific assessment (host application GEM; Cultivation-assessment type: soilless-surface water) are indicated by a white colour and that field which do not require input are indicated by a grey colour (and it is physically impossible to fill something in the field).

SPIN can be run in two different modes. Either stand-alone, in which case all properties are accessible and can all be filled in, or when started from a host application, in which case only the host-required properties (and in case of GEM also the Cultivation-assessment type specific substance properties) are accessible.

13) Fill in all properties for substance Pa1T2 according the datasheet given in Annex 2.

14) Save the substance by clicking the '√' button



15) Copy substance EXG0 to add a new substance to the SPIN database containing all default values.

16) Fill in all properties for substance M1T2 according the datasheet given in Annex 2.

17) Save the substance by clicking the '√' button

18) Select substance **Pa1T2** in the Browse substances table and click the metabolite scheme button:


19) Select the Recirculation water tab in the Metabolite screen

20) Click the '+' button. Note that the fields in the **Edit metabolites** part change from grey to white colour.

21) Select M1T2 from the pick list at the right hand site of field Metabolite

22) Fill in the fraction transformed (Annex 2) in the field of Fraction transformed

23) Save the metabolite scheme for M1T2 in recirculation water by clicking the '√' button

24) Repeat steps 19-23 for adding M1T2 as metabolite in surface water (select the Surface water tab in the Metabolite screen). If finished, close SPIN clicking the red button with the white cross in the upper right corner of the screen.

Assessments screen, section 'Edit Assessments' tab 'Assessment'

Substance

25) Select Pa1T2 from the picklist by clicking the box with the arrow at the right hand site of the field Substance.

Note that among others substances EXGE2 and EXGE3 are classified as 'incomplete' in the picklist. For these example substances not all necessary information for simulating soilless scenarios is provided to the database. Because the project you are working in now is a Soilless project, GEM will classify EXGE2 and EXGE3 classified as 'incomplete' for a Soilless project.

Applications

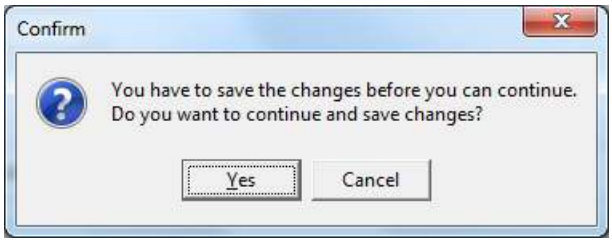
If the user chooses the option that calculations presume the reuse of filter water, he/she is given the choice of whether or not the application should be optimised with regard to discharge. Optimisation in this respect implies that the program will adjust the application date to a suitable date if the period between the specified application date and the discharge dates is shorter than allowed. This requires the user to specify the minimum interval between application and first subsequent discharge.

26) Check the thick box for 'Manage application with regard to discharge'

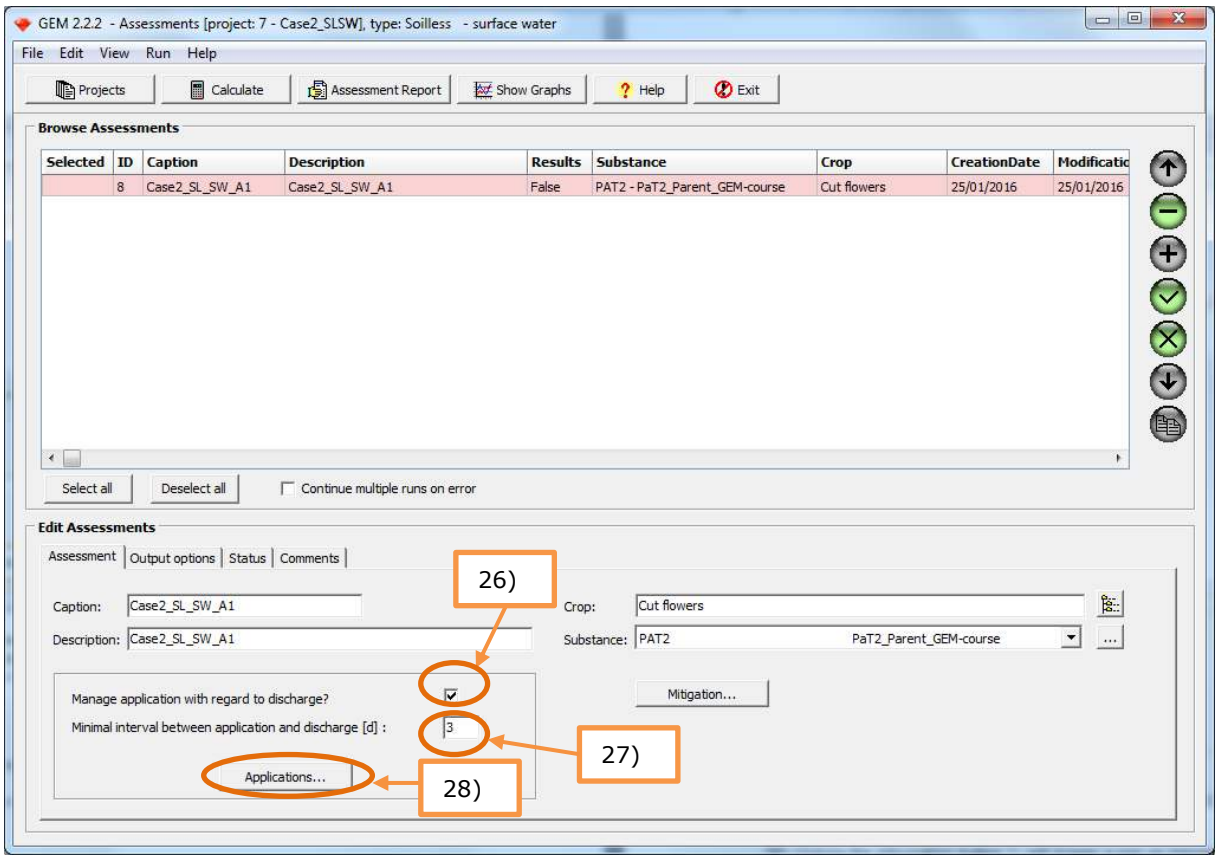
27) Fill in **3** days for the Minimum interval between application and discharge

28) Click on the button 'Applications''

29) The message box below appears. Click 'Yes



30) The GEM 2.2.2 Applications screen appears



31) Click the '+' button to add a new application event

The application data for Case 2 are found in Annex 2

32) Select the application type from the picklist by clicking the box with the arrow at the right hand site of the field Application Type.

33) Select the month and day of the application from the picklists by clicking the boxes with the arrow at the right hand site of the field Application Date.

34) Fill in the dosage in the field of Dosage

For the calculations with reuse of filter water, the user has specified the minimum number of days that preferably should occur between an application and the next subsequent discharge event. If the user, without realising it, chooses an application date which is too closely followed by a discharge date, the application is not allowed on that day. Hence, the program will automatically search for the nearest application date which fulfils the requirement of having the specified number of days prior to a discharge

event. For this reason, the user is given the possibility to enter the maximum number of days that the program may automatically adjust the application date in order to create sufficient time between application and discharge. The acceptable change in application date is specified as the number of days that the application date may be moved to an earlier or to a later date.

35) Set 'acceptable change in application data +/-' to 7 days (Note this is the maximum value possible)

36) Save the application by clicking the '√' button

Steps 31 – 36 need to be repeated for each application. It is usually quicker to use the 'copy' option for adding applications.

37) For adding additional applications click on the button:  (copy)

Note that the date of the copy of the application is automatically set to the following day.

38) Change the day of application: select the appropriate day from the picklists by clicking the box with the arrow at the right hand site of the field Application Date

39) Save the application by clicking the '√' button

If the program is not able to find an application date sufficiently far removed from subsequent discharge events, the user is warned by a text box on the right, with text in red stating that 'No solution found for one or more of your target application dates'. You may try an alternative application target date and/or search interval.'

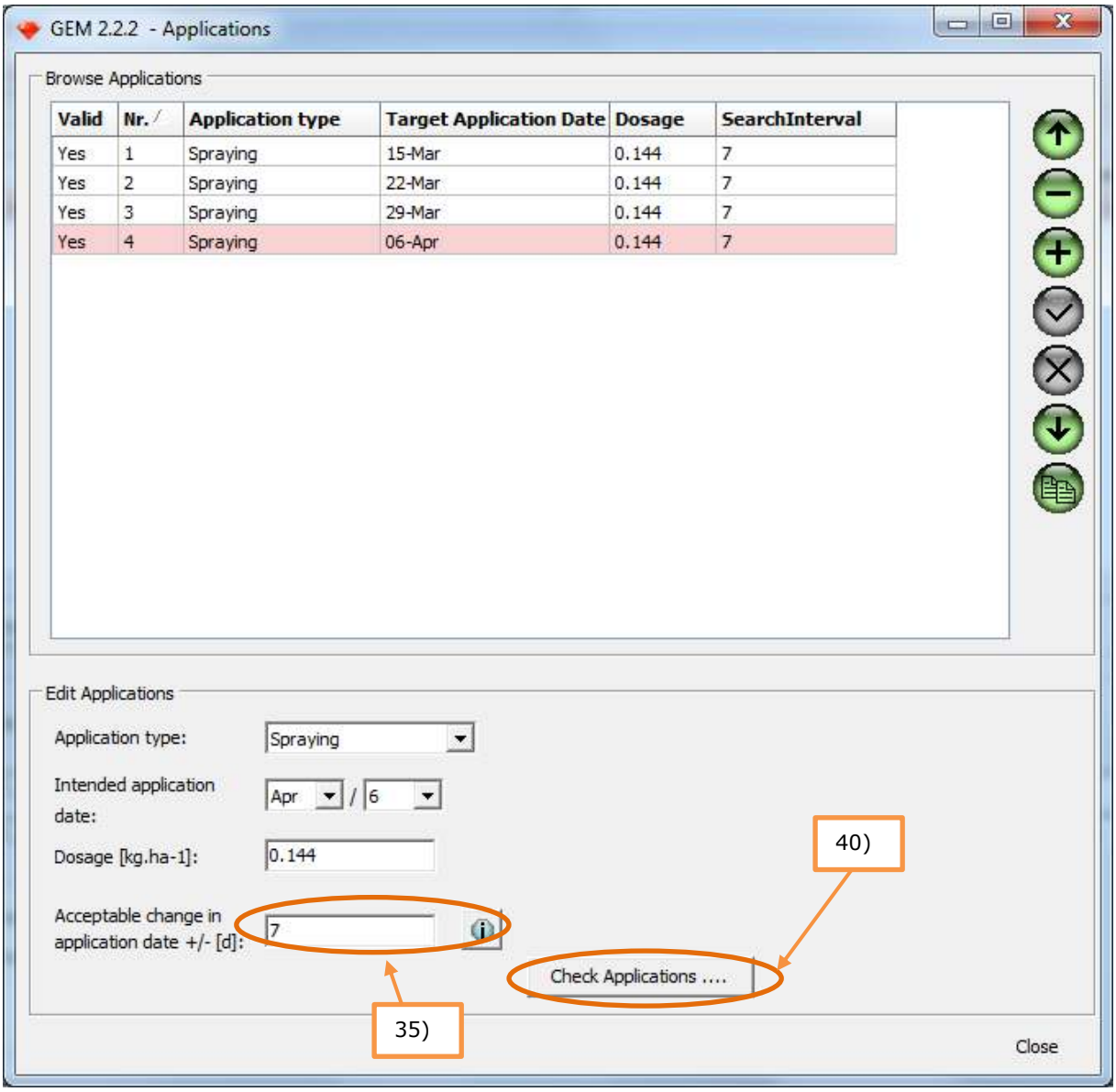
Regardless whether suitable application dates were found, with or without automatic adjustment of the dates by the program, the user can visualize the application dates by pressing the 'Check applications'

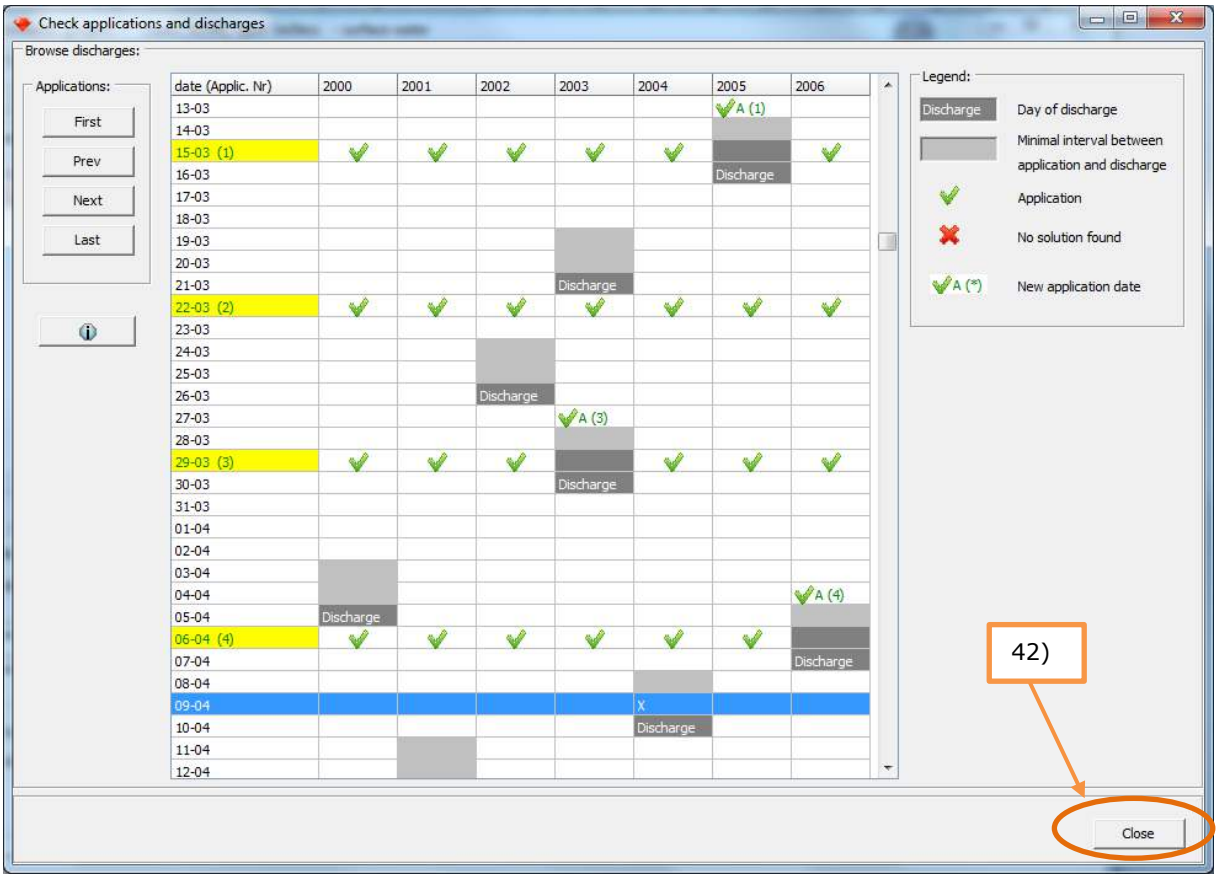
40) Click on the button 'Check Applications...'

41) Check that for each year and target application date that a solution is found. If this is not the case, adjust the target application date or lower the minimal interval between application and discharge (Assessments screen).

Note: the acceptable change in application date is already set to the maximum value of 7, lowering this value, will make it more difficult to find a solution.

You may fiddle around in order to see how this optimisation works.


GEM 2.2.2 - Applications
Browse Applications
Valid
Nr.
Application type
Target Application Date
Dosage
SearchInterval
Yes 1 Spraying 15-Mar 0.144 7
Yes 2 Spraying 22-Mar 0.144 7
Yes 3 Spraying 29-Mar 0.144 7
Yes 4 Spraying 06-Apr 0.144 7
Edit Applications
Application type:
Spraying
Intended application date:
Apr / 6
Dosage [kg.ha-1]:
0.144
Acceptable change in application date +/- [d]:
7
Check Applications ....
40)
35)
Close



Any user-chosen application date too close to a discharge, which cannot be adjusted by the program within the constraints of the 'acceptable change in application date' to allow an application anyway, will be marked in red on the Check applications and discharges screen and will make calculations impossible.

If the requirements for the minimal interval between application and discharge date are not met, no calculations can be performed for a 'reuse filter water' scenario. If under these circumstances the author selects the invalid assessment anyway, and tries to perform a calculation, the 'Finished' textbox will pop up immediately, without any calculations being performed for this assessment. GEM will continue with a next assessment provided that the 'Continue multiple runs on error' has been enabled.

42) Leave the Check applications and discharges screen by clicking the 'Close' button

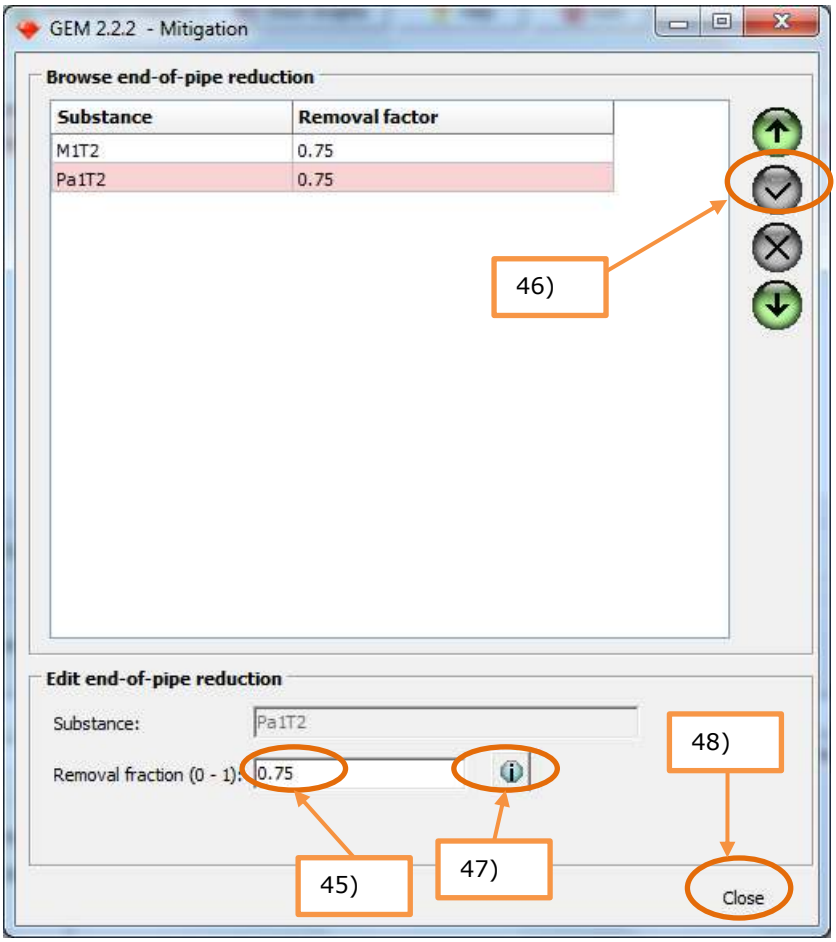
43) Leave the Application screen by clicking the 'Close' button

Mitigation

The mitigation option 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. 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.

44) Call the mitigation screen by clicking the mitigation button on the Assessment screen

The mitigation screen pops up. The record(s) for your substance(s) are already shown in the 'Browse end-of-pipe reduction' table. For changing the value of the removal fraction the relevant record needs to be selected by clicking on it in the table (in case of only one substance/record clicking on the record is not necessary).

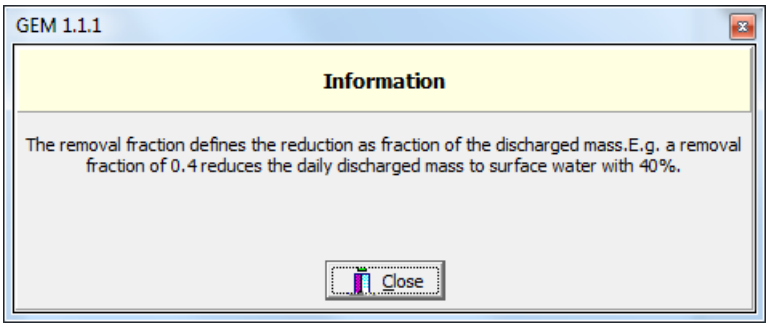


45) Fill in the value of the removal fraction (0.75) in the field of 'Removal fraction'. Do this for both parent and metabolite.

46) Save the removal fraction by clicking the '√' button

47) Clicking the information button 'i', will trigger a pop-up message giving information on the meaning of the removal fraction. Close the information screen clicking the 'Close' button.

48) Leave the Mitigation screen by clicking the 'Close' button



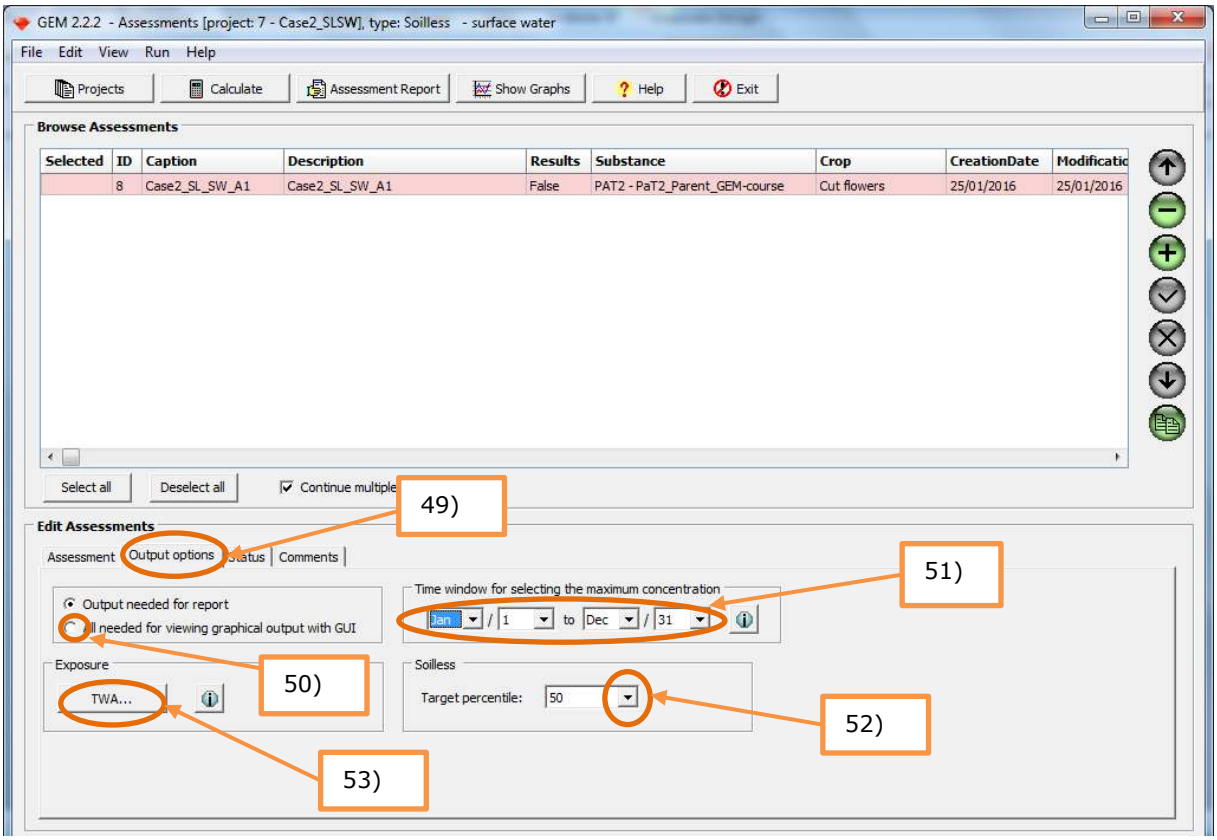
Assessments screen, section 'Edit Assessments', tab 'Output options'

Output options

49) Click in the section 'Edit Assessments' on the tab 'Output Options'

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. Viewing graphical output is possible only for surface water exposure assessments.

50) Select the radio button 'All needed for viewing graphical output with GUI'



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 of 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.

51) Play around with the dates in the field Time window for selecting the maximum concentration. You can select the appropriate days and months from the picklists by clicking the boxes with the arrows. However, set the values of the Time window back to January 1st – December 31st.

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

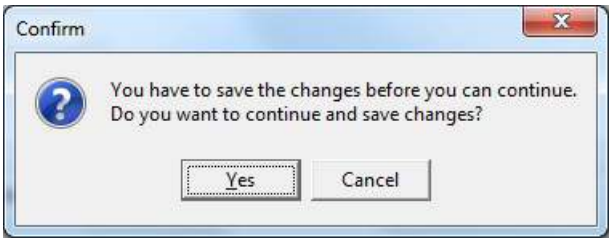
The endpoint of the exposure assessment, i.e. the Predicted Environmental Concentration (PEC), was defined as the target overall percentile annual peak concentration in an evaluation ditch with a length of 100 m. The target percentile (either a 50th or a 90th percentile) has not been decided yet by the risk managers

52) Select the 50th percentile concentration from the picklist by clicking the arrow at the right hand site of the field 'Target percentile'

53) Click the TWA button to add addition TWA records to the simulation

The software will by default calculate and report Time Weighted Average (TWA) concentrations calculated over periods of 7 days (TWA7d) and 21 days (TWA21d). 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. 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.

54) The message box below appears: Click the button 'Yes'



54) Click the '+' button to add a new TWA record

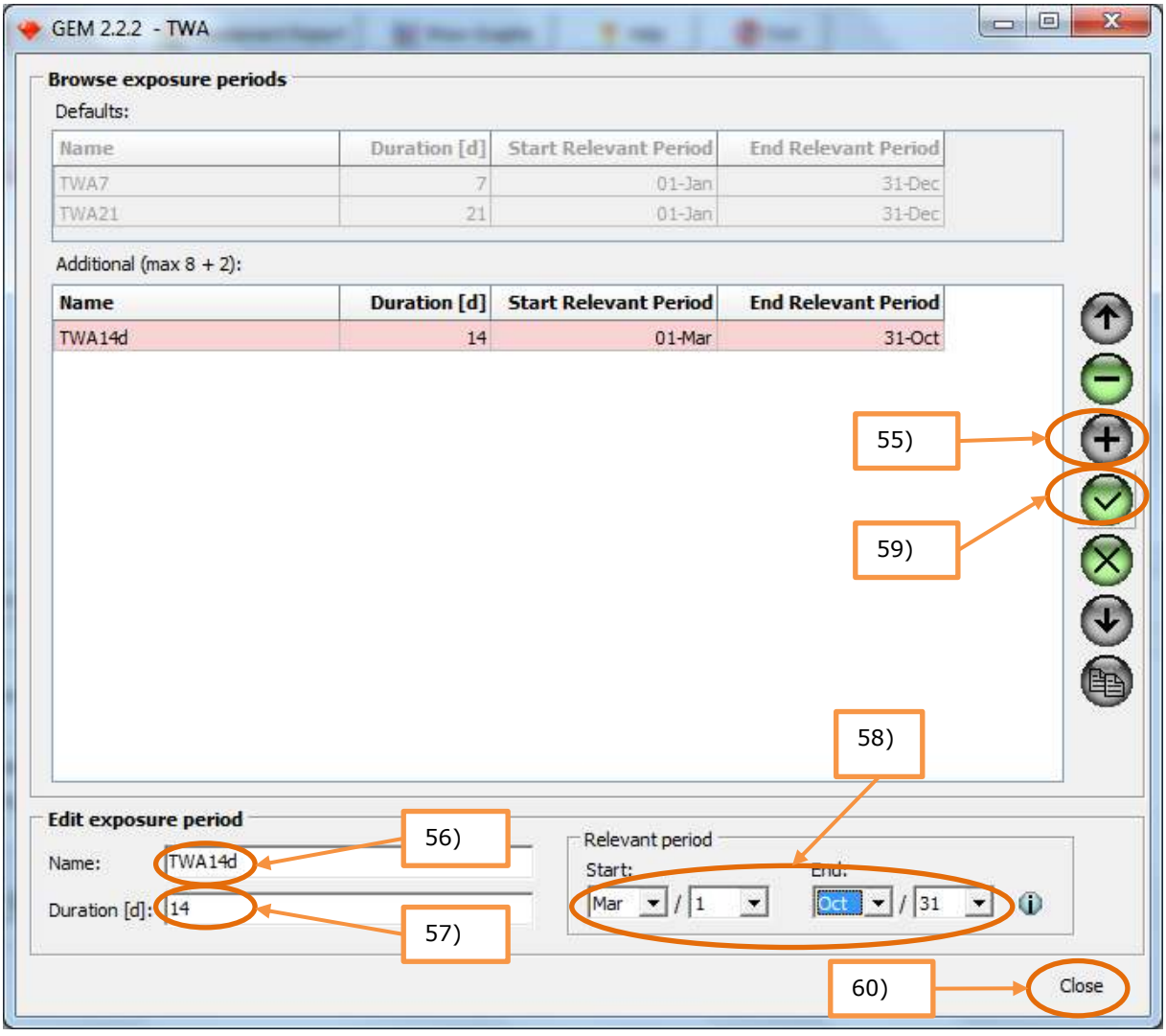
55) Fill in the name **'TWA14d'** in the field 'Name

56) Fill in a duration of **14** days in the field 'Duration'.

57) Change the relevant period to March 1st – October 31st : select the appropriate day from the picklists by clicking the boxes with the arrows in the field 'Relevant period'

58) Save the TWA record by clicking the '√' button

59) Leave the TWA screen by clicking the 'Close' button



At this moment all information needed for performing the simulations is entered into the software tools. The next step is to prepare the assessment(s) for simulation.

Three steps are necessary here:

1. Select the assessment(s) for simulation
2. Decide on whether to enable or disable 'Continue multiple runs on error'
3. Start the simulation(s)

60) Click the button 'Select all'. Note that the column 'Selected' in the Browse Assessments table is filled with 'Yes' indicating that the assessment is selected for simulation.

61) Disable 'Continue multiple runs on error' ; the tick box should be empty (in case of errors a notification will be given via a pop-up message)

62) Click the button 'Calculate'

The soilless-surface water exposure model train will start: 1.Water model (very quick simulation), 2. Substance model, 3. TOXSWA model

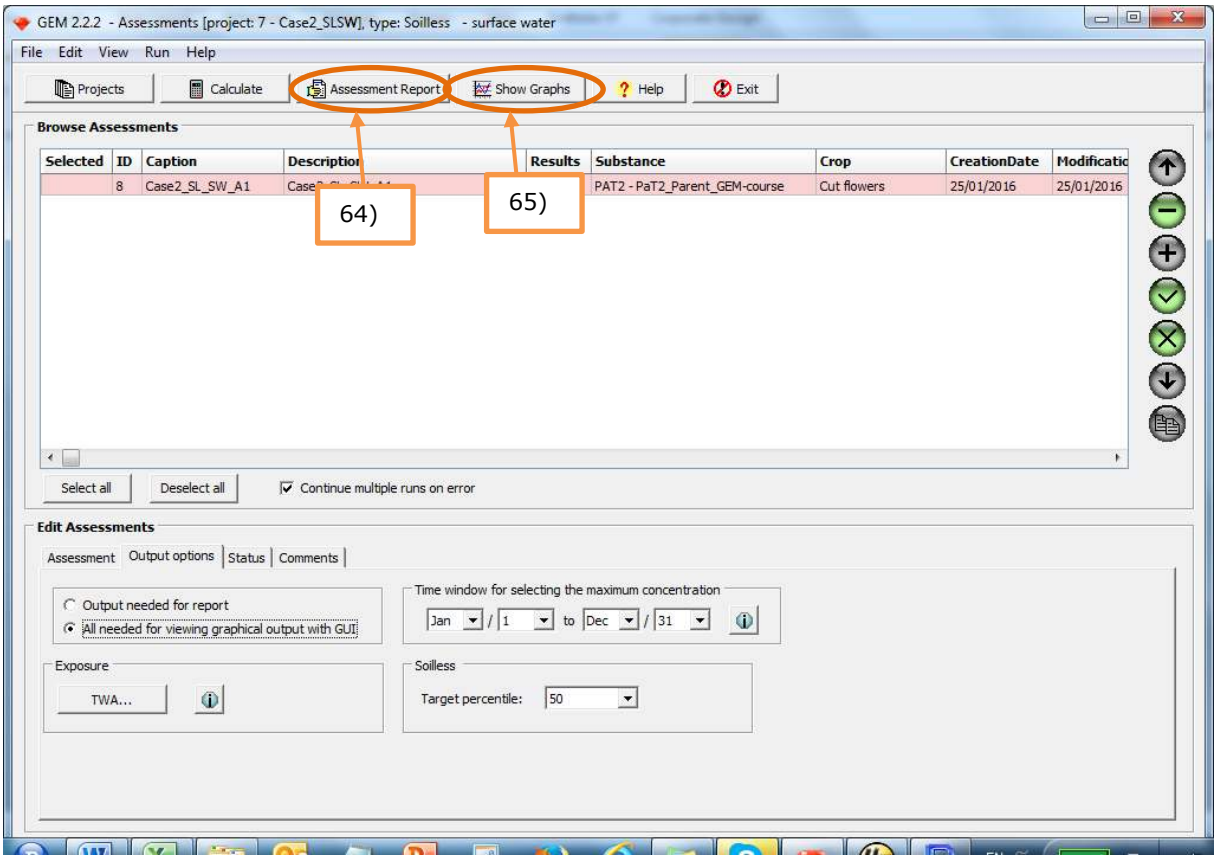
Once the simulation is successfully finished, the status of the assessment in the column Results in the table Browse Assessments will be set to True.

The simulation will take about an hour (30 minutes for each substance). The results of the simulation will be extracted from GEM and discussed tomorrow.

Time to relax!

Viewing results of the simulation of CASE 2

64) To open the assessment report click on the button 'Assessment Report'. The report (htm file) is automatically opened in the (default) web browser of your PC.



Open the assessment report and read out the 50th percentile concentration.

50th percentile PEC surface water Pa1T2----------

50th percentile PEC surface water M1T2----------

The corresponding Regulatory Acceptable Concentration for the parent substance is 420 µg/L (L(E)C50 invertebrates) times an assessment factor of 0.01. The corresponding Regulatory Acceptable Concentration for the Metabolite is 44 µg/L (L(E)C50 fish) times an assessment factor of 0.01. Would this substance be approved in case of 75% removal before discharge?

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65) To check out the graphs click on the button ‘Show graphs’.

    The graphs screen is opened.

66) Select a graph by selecting the corresponding radio button followed by clicking the ‘Show graph’ button.

Check out the graphs and think of how you could use these graphs in the evaluation of a dossier.

Annex 1 Pesticide properties and application data CASE 1

Substance

Parent substance PaT1 with 1 metabolite: M1T1 (soil)

Substance code: **Pa1T1**

Name: **Pa1T1-Parent_GEM-course**

Table A1.1 Substance properties **Pa1T1**

Property	value	unit	comment
Molar mass	511.2	$g.mol^{-1}$	
Half-life transformation in water	112	d	Measured at 20 °C Lower tier value
Half-life transformation in sediment	1000	d	Measured at 20 °C
Half-life transformation in soil	29.3	d	Measured at 20 °C
Coefficient of equilibrium sorption on organic matter in soil, sediment and suspended solids (Kom)	411.82	$L.kg^{-1}$	Measured at 20 °C
Reference concentration in liquid phase in soil/sediment/ suspended solids	1	$mg.L^{-1}$	
Freundlich exponent in soil/sediment/ suspended solids	0.98	-	
Saturated vapour pressure	4.E-6	Pa	Measured at 25 °C
Water solubility of substance	0.046	$mg.L^{-1}$	Measured at 20 °C
Half-life on crop canopy	10	d	Option lumped
Wash-off factor	100	m^{-1}	EFSA (2012a): 0.1 mm^{-1}
Coefficient for uptake by plants	0.5	-	
Coefficient for linear sorption on macrophytes	0	$L.kg^{-1}$	
L(E)C50 invertebrates (Acute)	1.3	$\mu g.L^{-1}$	
assessment factor:	100		0.01 times the L(E)C50

Defaults

Property	value	unit	comment
Molar enthalpy of vaporisation	95	kJ mol^{-1}	
Molar enthalpy of dissolution	27	kJ mol^{-1}	
Reference diffusion coefficient in water	4.3E-5	m^2 d^{-1}	Measured at 20 °C
Reference diffusion coefficient in air	0.43	m^2 d^{-1}	Measured at 20 °C
Molar enthalpy of sorption	0	kJ mol^{-1}	
Molar activation energy in soil	65.4	kJ mol^{-1}	
Molar activation energy in water	65.4	kJ mol^{-1}	
Molar activation energy in sediment	65.4	kJ mol^{-1}	
Exponent for the effect of liquid (Walker)	0.7	-	

Table A1.2 Substance properties **M1T1;** Name: **M1T1-Metabolite1_GEM-course**

Property	value	unit	comment
Molar mass	371.1	$g.mol^{-1}$	
Half-life transformation in water	53.9	d	Measured at 20 °C Lower tier value
Half-life transformation in sediment	1000	d	Measured at 20 °C
Half-life transformation in soil	13.0	d	Measured at 20 °C
Coefficient of equilibrium sorption on organic matter in soil, sediment and suspended solids (Kom)	45.26	$L.kg^{-1}$	Measured at 20 °C
Reference concentration in liquid phase in soil/sediment/ suspended solids	1	$mg.L^{-1}$	
Freundlich exponent in soil/sediment/ suspended solids	0.95	-	
Saturated vapour pressure	1.E-10	Pa	Measured at 20 °C
Water solubility of substance	3.9	$mg.L^{-1}$	Measured at 20 °C
Half-life on crop canopy	10	d	Option lumped
Wash-off factor	100	m^{-1}	EFSA (2012a): 0.1 mm^{-1}
Coefficient for uptake by plants	0.5	-	

Coefficient for linear sorption on macrophytes	0	$L.kg^{-1}$	
Formation fraction in soil	0.318	-	
L(E)C50 Fish (Acute)	1100	$\mu g.L^{-1}$	
assessment factor:	100		0.01 times the L(E)C50

Defaults

Property	value	unit	comment
Molar enthalpy of vaporisation	95	kJ mol^{-1}	
Molar enthalpy of dissolution	27	kJ mol^{-1}	
Reference diffusion coefficient in water	4.3E-5	m^2 d^{-1}	Measured at 20 °C
Reference diffusion coefficient in air	0.43	m^2 d^{-1}	Measured at 20 °C
Molar enthalpy of sorption	0	kJ mol^{-1}	
Molar activation energy in soil	65.4	kJ mol^{-1}	
Molar activation energy in water	65.4	kJ mol^{-1}	
Molar activation energy in sediment	65.4	kJ mol^{-1}	
Exponent for the effect of liquid (Walker)	0.7	-	

EFSA Scientific Panel on Plant Protection Products and their Residues (PPR), 2012a. Scientific Opinion on the science behind the guidance for scenario selection and scenario parameterisation for predicting environmental concentrations of plant protection products in soil. EFSA Journal 2012;10(2):2562 [76 pp.].

Mitigation: not applicable for soil-bound projects/assessments

Applications:

Table A1.3 Applications scheme assessment CASE 1:

crop: **cut flowers (DTG code 7.2.1.2)**

timing	Number of applications	Min. interval between applications (d)	method	Dosage ($kg\ ha^{-1}$)	Fraction intercepted (-)	Instruction
Mar-Jun	2	15	To the crop canopy	0.06	0.5	Select one of the months and give the first application on the 15th
Sep-Nov	2	15	To the crop canopy	0.075	0.5	

Annex 2 Pesticide properties and application data CASE 2

Substance

Parent substance Pa1T2 with 1 metabolite: M1T2 (recirculation water)

Substance code: **Pa1T2**

Name: **Pa1T2-Parent_GEM-course**

Table A2.1 Substance properties **Pa1T2**

Property	value	unit	comment
Molar mass	300.4	$g.mol^{-1}$	
Half-life transformation in surface water	0.25	d	Measured at 20 °C
Half-life transformation in sediment	1000	d	Measured at 20 °C
Half-life transformation in recirculation water, including the disinfection tank	0.8	d	Measured at 25 °C and pH 7
Half-life transformation in greenhouse air	1.0	d	Measured at 20 °C
Half-life transformation in substrate	1.0	d	
Coefficient of equilibrium sorption on organic matter in soil, sediment and suspended solids (Kom)	1778	$L.kg^{-1}$	
Reference concentration in liquid phase in sediment/ suspended solids	1	$mg.L^{-1}$	
Freundlich exponent in sediment/ suspended solids	0.9	-	
Saturated vapour pressure	1.33^{E}-5	Pa	Measured at 25 °C
Water solubility of substance	3.8	$mg.L^{-1}$	Measured at 20 °C
Octanol-water coefficient	2512	-	
Half-life transformation on greenhouse floor	100	d	Measured at 20 °C
Half-life on crop canopy	10	d	Option lumped
Coefficient for linear sorption on macrophytes	0	$L.kg^{-1}$	
L(E)C50 invertebrates (Acute)	420	$\mu g.L^{-1}$	
Assessment factor	100		0.01 times the L(E)C50

Defaults

Property	value	unit	comment
Molar activation energy in greenhouse air	45	kJ mol^{-1}	
Molar activation energy in recirculation water	65.4	kJ mol^{-1}	
Molar enthalpy of vaporisation	95	kJ mol^{-1}	
Molar enthalpy of dissolution	27	kJ mol^{-1}	
Reference diffusion coefficient in water	4.3E-5	m^2 d^{-1}	Measured at 20 °C
Reference diffusion coefficient in air	0.43	m^2 d^{-1}	Measured at 20 °C
Molar activation energy in water	65.4	kJ mol^{-1}	
Molar activation energy in sediment	65.4	kJ mol^{-1}	

Table A2.2 Substance properties **M1T2;** Name: **M1T2-Metabolite2_GEM-course**

Property	value	unit	comment
Molar mass	298.3	$g.mol^{-1}$	
Half-life transformation in surface water	1	d	Measured at 20 °C
Half-life transformation in sediment	1000	d	Measured at 20 °C
Half-life transformation in recirculation water, including the disinfection tank	1.2	d	Measured at 25 °C and pH 7
Half-life transformation in greenhouse air	1.0	d	Measured at 20 °C
Half-life transformation in substrate	6.0	d	Measured at 20 °C
Coefficient of equilibrium sorption on organic matter in soil, sediment and suspended solids (Kom)	5124	$L.kg^{-1}$	
Reference concentration in liquid phase in sediment/ suspended solids	1	$mg.L^{-1}$	
Freundlich exponent in sediment/ suspended solids	0.9	-	
Saturated vapour pressure	1E-10	Pa	Measured at 25 °C
Water solubility of substance	100	$mg.L^{-1}$	Measured at 25 °C
Octanol-water partitioning coefficient	1260	-	

Half-life transformation on greenhouse floor	100	d	Measured at 20 °C
Half-life on crop canopy	10	d	Option lumped
Coefficient for linear sorption on macrophytes	0	$L.kg^{-1}$	
Formation fraction in recirculation water (hydrolysis at pH 7)	0.585	-	
Formation fraction in surface water	0.328		
L(E)C50 fish (Acute)	44	$\mu g.L^{-1}$	
assessment factor	100		0.01 times the L(E)C50

Defaults

Property	value	unit	comment
Molar activation energy in greenhouse air	45	kJ mol^{-1}	
Molar activation energy in recirculation water	65.4	kJ mol^{-1}	
Molar enthalpy of vaporisation	95	kJ mol^{-1}	
Molar enthalpy of dissolution	27	kJ mol^{-1}	
Reference diffusion coefficient in water	4.3E-5	m^2 d^{-1}	Measured at 20 °C
Reference diffusion coefficient in air	0.43	m^2 d^{-1}	Measured at 20 °C
Molar activation energy in water	65.4	kJ mol^{-1}	
Molar activation energy in sediment	65.4	kJ mol^{-1}	

Mitigation: removal fraction = 0.75

Applications:

Table A2.3 Applications scheme assessment CASE 2:

crop: **cut flowers (DTG code 7.2.1.2)**

The minimum interval between application and discharge should be at least 3 days

timing	Number of applications	Min. interval between applications (d)	method	Dosage (kg ha^{-1})	Instruction
March-Aug	4	7	spraying	0.144	Select one of the months and give the first application on the 15th

Annex 3 DTG LIST in Crops screen of GEM 2.2.2

In the Dutch authorisation process for the use of a plant protection product, an authorisation can be requested for crops that are listed in the "Definitielijst Toepassingsgebieden Gewasbeschermings-middelen" (Definition list of areas of application for plant protection products; in this report referred to as the DTG-list). The DTG-list has a hierarchical structure containing 4 categories for subdivision: Cultivation categories, crop categories, crop sub categories and crops (Figure A3.1).

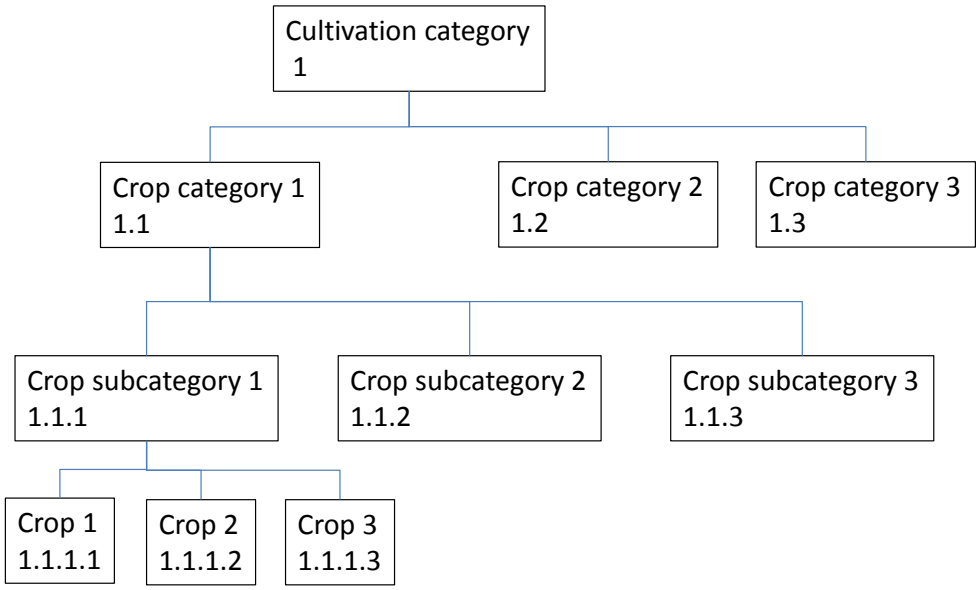


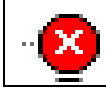
Figure A3.1 hierarchical structure of the DTG-list

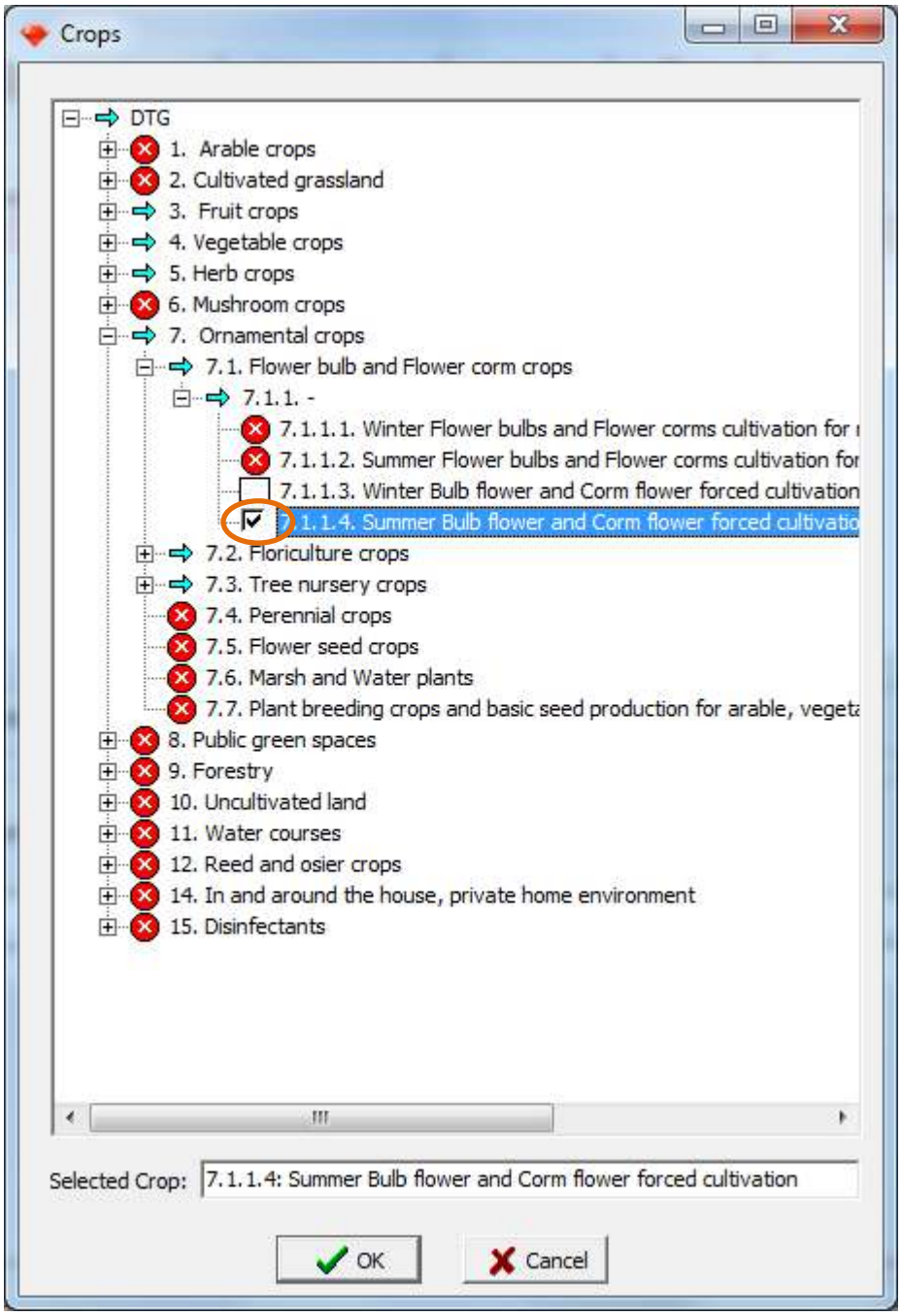
The complete DTG-list is incorporated in the GEM software tool.

Below an example is shown of the hierarchical structure:

1.	cultivation categories	7. Ornamental crops
2.	crop categories	7.1 Flower bulb and flow corm crops
3.	crop sub categories	7.1.1 -
4.	crops	7.1.1.3 Winter bulb flower and corm flower forced cultivation

The DTG list in the screen 'Crops' of GEM shows different symbols which are explained below:

	Expanding the DTG list
	Closing the corresponding category
	The corresponding DTG category contains lower levels available for selection indicating that all/some of these lower levels are relevant for your particular assessment (in GEM determined by the chosen Cultivation-assessment type)
	The corresponding DTG category contains lower levels that are NOT available for selection indicating that all of these lower levels are NOT relevant for your particular assessment (in GEM determined by the chosen Cultivation-assessment type)



- The crop relevant for your case can be selected by clicking the white empty box. A crop is selected when a '√' symbol appears in the box and the selected crop is indicated in the field of 'Select Crop' at the bottom of the Crops screen.
- Click the 'OK' button to save the selected crop for your particular assessment

Annex 4 Answers GEM Hands-on training cases

1. *CASE 1: Soil-bound groundwater;*

Substance: **Pa1T1 (M1T1)**
crop: **cut flowers (DTG code 7.1.2.2)**

timing	Number of applications	Min. interval between applications (d)	method	Dosage (kg ha^{-1})	Fraction intercepted (-)	Instruction
Mar-Jun	2	15	To the crop canopy	0.06	0.5	Select one of the months and give the first application on the 15th
Sep-Nov	2	15	To the crop canopy	0.075	0.5	

Applications dates	90th percentile PEC groundwater Pa1T1 (ug/L)	90th percentile PEC groundwater M1T1 (ug/L)
15 Mar, 30 Mar, 15 Sep, 30 Sep	0.000030	0.015599
15 Mar, 30 Mar, 15 Oct, 30 Oct	0.000029	0.015032
15 Mar, 30 Mar, 15 Nov, 30 Nov	0.000028	0.014704
15 Apr, 30 Apr, 15 Sep, 30 Sep	0.000029	0.015668
15 Apr, 30 Apr, 15 Oct, 30 Oct	0.000028	0.015099
15 Apr, 30 Apr, 15 Nov, 30 Nov	0.000028	0.014770
15 May, 30 May, 15 Sep, 30 Sep	0.000030	0.015910
15 May, 30 May, 15 Oct, 30 Oct	0.000028	0.015338
15 May, 30 May, 15 Nov, 30 Nov	0.000028	0.015007
15 Jun, 30 Jun, 15 Sep, 30 Sep	0.000029	0.015936
15 Jun, 30 Jun, 15 Oct, 30 Oct	0.000028	0.015362
15 Jun, 30 Jun, 15 Nov, 30 Nov	0.000028	0.015029

2. *CASE 1: Soil-bound surface water*

Substance: **Pa1T1 (M1T1)**
crop: **cut flowers (DTG code 7.1.2.2)**

timing	Number of applications	Min. interval between applications (d)	method	Dosage (kg ha^{-1})	Fraction intercepted (-)	Instruction
Mar-Jun	2	15	To the crop canopy	0.06	0.5	Select one of the months and give the first application on the 15th
Sep-Nov	2	15	To the crop canopy	0.075	0.5	

Applications dates	90th percentile PEC surface water Pa1T1 (ug/L)	90th percentile PEC surface water M1T1 (ug/L)
15 Mar, 30 Mar, 15 Sep, 30 Sep	0.04664	0.03971
15 Mar, 30 Mar, 15 Oct, 30 Oct	0.04839	0.04017
15 Mar, 30 Mar, 15 Nov, 30 Nov	0.05013	0.04098
15 Apr, 30 Apr, 15 Sep, 30 Sep	0.05996	0.04295
15 Apr, 30 Apr, 15 Oct, 30 Oct	0.06172	0.04341
15 Apr, 30 Apr, 15 Nov, 30 Nov	0.06348	0.04423
15 May, 30 May, 15 Sep, 30 Sep	0.08387	0.04472
15 May, 30 May, 15 Oct, 30 Oct	0.08566	0.04527
15 May, 30 May, 15 Nov, 30 Nov	0.08744	0.04608
15 Jun, 30 Jun, 15 Sep, 30 Sep	0.05459	0.03840
15 Jun, 30 Jun, 15 Oct, 30 Oct	0.05571	0.03894
15 Jun, 30 Jun, 15 Nov, 30 Nov	0.05705	0.03974

The corresponding Regulatory Acceptable Concentration for the parent substance is 1.3 µg/L (L(E)C50 invertebrates) times an assessment factor of 0.01. The corresponding Regulatory Acceptable Concentration for the metabolite is 1100 µg/L (L(E)C50 fish) times an assessment factor of 0.01.

3. CASE 2: Soilless surface water

Substance: **Pa1T2 (M1T2)**

Crop: **cut flowers (DTG code 7.1.2.2)**

The minimum interval between application and discharge: **3 days**
Acceptable change in application date: **7 d**

timing	Number of applications	Min. interval between applications (d)	method	Dosage (kg ha^{-1})	Instruction
March-Aug	4	7	spraying	0.144	Select one of the months possible and give the first application on the 15th

Applications dates	50th percentile PEC surface water Pa1T2 (ug/L)	50th percentile PEC surface water M1T2 (ug/L)
15 Mar, 22 Mar, 29 Mar, 5 Apr	0.3514	0.5868
15 Apr, 22 Apr, 29 Apr, 6 May	0.2196	0.4086
15 May, 22 May, 29 May, 5 Jun	0.1883	0.3459
15 Jun, 22 Jun, 29 Jun, 6 Jul	0.08330	0.1613
15 Jul, 22 Jul, 29 Jul, 5 Aug	0.04908	0.09029

The corresponding Regulatory Acceptable Concentration for the parent substance is 420 µg/L (L(E)C50 invertebrates) times an assessment factor of 0.01. The corresponding Regulatory Acceptable Concentration for the Metabolite is 44 µg/L (L(E)C50 fish) times an assessment factor of 0.01.