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



• The GEM 2.2.2 – Project screen is opened:

	ise Projects					
D	Caption	Description	CultivationType	CreationDate	ModificationDate	
1	ExProject1	Example Project 1 soilless culti	Soilless - surface water	22/01/2016 10:13:33	22/01/2016 10:13:33	1
2	ExProject2	Example project 2 soil-bound-	Soil-bound - surface water	22/01/2016 10:13:33	22/01/2016 10:13:33	1
3	ExProject3	Example project 3 soil-bound -	Soil-bound - ground water	22/01/2016 10:13:33	22/01/2016 10:13:33	
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lit I Gen	Projects eral Comments Comments		CreationDate:	22/01/2016	¥	
lit I ien Ca De	Projects eral Comments ption: ExProject1 scription: Example Pr	roject 1 soilless cultivation-surfac	CreationDate: Te wat ModificationDate:	22/01/2016	× ×	
lit I ien De Ca	Projects eral Comments ption: ExProject1 scription: Example Pr Cultivation - assessment Solless - surface wa Soll-bound - surface v Soll-bound - ground v	t roject 1 soilless cultivation-surfac t type: ter water water water C 2018 C 2018	CreationDate: ModificationDate: temission reference period: -2017 2017 (filter water reused) 2020 (filter water reused)	22/01/2016 22/01/2016	<u>v</u> v	

• 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.

ouse i roje	cts					
ID Caption	Des	cription	CultivationType	CreationDate	ModificationDate	6
1 ExProject:	1 Exan	nple Project 1 soilless culti	Soilless - surface water	22/01/2016 10:13:33	22/01/2016 10:13:33	
2 ExProject2	2 Exan	mple project 2 soil-bound-:	Soil-bound - surface water	22/01/2016 10:13:33	22/01/2015 10:13:33	6
3 ExProject3	3 Exan	mple project 3 soil-bound -	Soil-bound - ground water	22/01/2016 10:13:33	22/01/2016 10:13:33	
				1)		
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dit Projects General Com Caption:	ments		CreationDate:	22/01/2016	×	
dit Projects General Com Caption: Description:	ments ExProject1 Example Project	1 soilless cultivation-surfac	CreationDate: e wat ModificationDate:	22/01/2016 22/01/2016	<u>×</u>	
dit Projects General Com Caption: Description: Cultivation Colless C Soil-bou C Soil-bou	ments EXProject 1 EXProject 1 - assessment type: - surface water nd - surface water nd - ground water	1 soilless cultivation-surfac Nutrient C 2015 C 2018 C 2018	CreationDate: We wat ModificationDate: emission reference period: -2017 -2017 (filter water reused) -2020 -2020 (filter water reused)	22/01/2016 22/01/2016	× ×	

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



wse S	iubstances					
ocked	SubstanceCode / Na	ne		CreationDate	LastModified	6
8	EXGE0 GEM	1 default values for soil-bou	ind SW and soilless	18/01/2016 15:13:58	18/01/2016 15:13:58	
8	EXGE1 GEM	1 example substance for so	il-bound SW and soilless	13/11/2014 14:26:02	13/11/2014 14:26:02	6
8	EXGE2 exa	mple substance for soil-bou	ind GW	13/11/2014 14:26:02	13/11/2014 14:26:02	0
8	EXGE3 exa	mple metabolite for soil-bou	and GW	13/11/2014 14:26:02	13/11/2014 14:26:02	6
9	EXSW0 FOO	CUS surface water Default_	values	25/06/2015 09:16:09	25/06/2015 09:16:09	
8	EXSW1 FOO	CUS surface water Example	_Sub_A	25/06/2015 09:16:09	25/06/2015 09:16:09	6
8	EXSW2 FOO	CUS surface water Example	_Sub_H	25/06/2015 09:16:09	25/06/2015 09:16:09	
8	EXSW3 FOO	CUS surface water Example	_Sub_6	25/06/2015 09:16:09	25/06/2015 09:16:09	6
8	EXSW4 FOO	CUS surface water Example	_Sub_6m_sw, soil metabolite from 6_sw	25/06/2015 09:16:09	25/06/2015 09:16:09	V 1
t Subs	tance					
it Subs	stance	rocesses				
it Subs ieneral Substa	s tance Sorption Transformation Crop p anceCode:	rocesses				
it Subs ieneral Substa Name:	s tance Sorption Transformation Crop ; anceCode:	rocesses EXSW1 FOCUS surface wat	er Example_Sub_A			
it Subs ieneral Substa Name: Molar	stance Sorption Transformation Crop ; anceCode: : mass (g mol-1):	FOCUS surface wat	er Example_Sub_A			
it Subs ieneral Substa Name: Molar Satura	stance Sorption Transformation Crop ; anceCode: : mass (g mol-1): ated vapour pressure (Pa):	FOCUS surface wat 300 1E-7	er Example_Sub_A	20	D	
it Subs ieneral Substa Name: Molar Satura Molar	tance Sorption Transformation Crop p anceCode: : mass (g mol-1): ated vapour pressure (Pa): enthalpy of vaporisation (kJ mol-1):	rocesses EXSW1 FOCUS surface wat 300 1E-7 95	er Example_Sub_A	20	D	
it Subs ieneral Substa Name: Molar Satura Molar Solubil	tance Sorption Transformation Crop p anceCode: : mass (g mol-1): ated vapour pressure (Pa): enthalpy of vaporisation (kJ mol-1): lity in water (mg L-1):	rocesses EXSW1 FOCUS surface wat 300 1E-7 95 1	er Example_Sub_A () () Measured at (°C): () Measured at (°C):	20 (20)	D	
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it Substa Substa Name: Molar Satura Solubil Molar Refere d-1):	stance sorption Transformation Crop ; anceCode: : mass (g mol-1): ated vapour pressure (Pa): enthalpy of vaporisation (kJ mol-1): ity in water (mg L-1): enthalpy of dissolution (kJ mol-1): ence diffusion coefficient in water (m	rocesses EXSW1 FOCUS surface wat 300 1E-7 95 1 27 27 4.3E-5	er Example_Sub_A () () Measured at (°C): () Measured at (°C): () Peference temperature (°C):	20 (20 (D	
it Subst ieneral Substz Molar Satura Solubil Molar Refere d-1): Refere	itance sorption Transformation Crop ; anceCode: : mass (g mol-1): ated vapour pressure (Pa): enthalpy of vaporisation (kJ mol-1): lity in water (mg L-1): enthalpy of dissolution (kJ mol-1): ence diffusion coefficient in water (m2 d	rocesses EXSW 1 FOCUS surface wat 300 1E-7 95 1 27 2 4.3E-5 -1): 0.43	er Example_Sub_A (1) (1) (2) (2) (2) (2) (3) (4) (5) (5) (5) (5) (6) (7) (7) (7) (7) (7) (7) (7) (7	20 20 20	D D	

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
- elete 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
 - yopen 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...'

	Woder versions				
OCKEL	CubatanaeCode Nar	ne	CreationDate	LastModified	16
	PaT1 PaT	1_Parent_GEM-course	22/01/2016 15:54:23	22/01/2016 15:54:32	
9	EXGE0 GEM	I default values for soil-bound SW and soilless	18/01/2016 15:13:58	18/01/2016 15:13:58	6
8	EXGE1 GEM	example substance for soil-bound SW and soilless	13/11/2014 14:26:02	13/11/2014 14:26:02	
8	EXGE2 exa	mple substance for soil-bound GW	13/11/2014 14:26:02	13/11/2014 14:26:02	6
8	EXGE3 exa	mple metabolite for soil-bound GW	13/11/2014 14:26:02	13/11/2014 14:26:02	
9	EXSW0 FOO	US surface water Default_values	25/06/2015 09:16:09	25/06/2015 09:16:09	
8	EXSW1 FOO	:US surface water Example_Sub_A	25/06/2015 09:16:09	25/06/2015 09:16:09	
8	EXSW2 FOO	:US surface water Example_Sub_H	25/06/2015 09:16:09	25/06/2015 09:16:09	6
8	EXSW3 FOO	CUS surface water Example_Sub_6	25/06/2015 09:16:09	25/06/2015 09:16:09	V
9	EXSW4 FOO	US surface water Example_Sub_6m_sw, soil metabolite from 6_sw	v 25/06/2015 09:16:09	25/06/2015 09:16:09	6
it Subs	stance		3)		
lit Subs General Substa	stance Sorption Transformation Crop p anceCode:	rocesses	3)	•	
lit Subs General Substa Name:	stance Sorption Transformation Crop p anceCode:	FOCESSES EXIGED GEM default values for soll-bound SW and solless	3)	4)	
lit Subs General Substa Name: Molar	stance Sorption Transformation Crop p anceCode: : mass (g mol-1):	FOCESSES EXIGED GEM default values for soil-bound SW and soilless <no given="" value=""></no>	3)	-4)	
lit Subs General Substa Name: Molar Satura	stance Sorption Transformation Crop p anceCode: : mass (g mol-1): ated vapour pressure (Pa):	EXGE0 GEM default values for soll-bound SW and soilless <no given="" value=""> <no given="" value=""> <no given="" value=""> <no given="" value=""> <no given="" value=""></no></no></no></no></no>	3)	-4)	
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lit Subst General Name: Molar Satura Molar Solubi	stance Sorption Transformation Crop p anceCode: : mass (g mol-1): ated vapour pressure (Pa): enthalpy of vaporisation (kJ mol-1): lity in water (mg L-1):	EXGE0 GEM default values for soll-bound SW and soilless <no given="" value=""> <no given="" value=""></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no>	3) 20 20 (j)	4)	
lit Subst General Name: Molar Satura Molar Solubi Molar	stance Sorption Transformation Crop p anceCode: : mass (g mol-1): ated vapour pressure (Pa): enthalpy of vaporisation (kJ mol-1): lity in water (mg L-1): enthalpy of dissolution (kJ mol-1):	EXGE0 GEM default values for soll-bound SW and soilless <no given="" value=""> <novalue given=""><td>3)</td><td>4)</td><td></td></novalue></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no>	3)	4)	
lit Subst General Subst Name: Molar Satura Solubi Molar Refere d-1):	stance Sorption Transformation Crop p anceCode: : mass (g mol-1): ated vapour pressure (Pa): enthalpy of vaporisation (kJ mol-1): lity in water (mg L-1): enthalpy of dissolution (kJ mol-1): ence diffusion coefficient in water (m	EXGE0 GEM default values for soll-bound SW and soilless <no given="" value=""> <td></td><td>4)</td><td></td></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no></no>		4)	
lit Subst Seneral Subst Name: Molar Satura Molar Solubi Molar Refer d-1): Refere	stance Sorption Transformation Crop p anceCode: : mass (g mol-1): ated vapour pressure (Pa): enthalpy of vaporisation (kJ mol-1): enthalpy of dissolution (kJ mol-1): ence diffusion coefficient in water (m ence diffusion coefficient in air (m2 d	EXGE0 GEM default values for soll-bound SW and soilless <no given="" value=""> <td>3) 20 20 (j) 20 (j)</td><td>4)</td><td></td></no></no></no></no></no></no></no></no>	3) 20 20 (j) 20 (j)	4)	

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.

Model Versions	×
Select model versions	
TOXSWA for DRAINBOW PEARL for DRAINBOW PEARL for SOIL_PEARL TOXSWA for GEM Substance emission model for GEM	6)
MACRO for FOCUS SWASH 4.2 TOXSWA for FOCUS TOXSWA 4.4.2 MACRO for FOCUS SWASH 5.3 PRZM for FOCUS SWASH 5.3	7)
	OK Cancel

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.

Browse r 12) es formed in soil compa	rtment Fraction transformed	
M1T1 (M1T1_Metabolite1T1_GEM-course)	0.318	
Edit metabolites formed in soil compartm	ent abolite 1T 1_GEM-course)	

- 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 ' $\sqrt{'}$ 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



• 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 ' $\sqrt{}'$ button
- 23) Select Case1-SBSW in the Browse Projects table and click on the copy ¹⁰⁰ 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 ' $\sqrt{}'$ button

owse Projects				
D Caption	Description	CultivationType	CreationDate	ModificationDate
1 ExProject1	Example Project 1 soilless culti	Soilless - surface water	22/01/2016 10:13:33	22/01/2016 10:13:33
2 ExProject2	Example project 2 soil-bound-:	Soil-bound - surface water	22/01/2016 10:13:33	22/01/2016 10:13:33
3 ExProject3	Example project 3 soil-bound -	Soil-bound - ground water	22/01/2016 10:13:33	22/01/2016 10:13:33
5 Case 1_SBSW	Case 1 Soilbound Surface wab	Soil-bound - surface water	24/01/2016 14:49:33	19) 50:05
6 Case1_SBGW	Case1 Soilbound Groundwate	Soil-bound - ground water	24/01/2016 14:50:14	50:24
it Projects	1			J
it Projects eneral Comments Caption: Case Description: Case	21_SBGW 21), 25)	CreationDate: ModificationDate:	24/01/2016 24/01/2016	
it Projects eneral Comments Caption: Case Description: Case Cultivation - asses C Soilless - surf C Soil-bound - su Soil-bound - gr	21), 25) 21 Soilbound Groundwater sement type: rface water ound water	CreationDate: ModificationDate: emission reference period: - 20) :er water reused) -2020	24/01/2016 24/01/2016	27)

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'

Selected ID Caption Description Results Substance Crop CreationDate cnot available > cnot available > <t< th=""><th>Modificatio</th></t<>	Modificatio
cnot available > <not available=""> <not a<="" th=""><th>riouncauc (T</th></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not></not>	riouncauc (T
	<not availab<="" td=""></not>
Select all Deselect all No assessments; add an assessment by clicking on the plus-sign on the right hand side. Hide this message next time? Yes	,
In Assessments	
Caption: Crop:	
Caption: Crop: Description: Substance:	·
Caption: Crop: Crop: Crop: Substance:	<u> </u>

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.

Crops	
⊟-⇒ DTG	1
🕀 🔯 1. Arable crops	
🕀 🐼 2. Cultivated grassland	
⊕ ⇒ 3. Fruit crops	
⊕ ➡ 4. Vegetable crops	
⊕ ⇒ 5. Herb crops	
🕀 🐼 6. Mushroom crops	
□ ⇒ 7. Ornamental crops	
7.1. Flower bulb and Flower corm crops	
🔁 🔿 7.2. Floriculture crops	
⊡	
7.2.1.2. Cut flowers	
7.2.1.3. Forced shrubs	
7.2.1.4. Cut green	
7.4. Perennial crops	
7.5. Flower seed crops	
7.6. Marsh and Water plants	ar text rest in the
7.7. Plant breeding crops and basic seed produc	tion for arable, vegeta
+ 8. Public green spaces	
9. Forestry	
10. Uncultivated land	
11. Water courses	
12. Reed and osier crops	
14. In and around the house, private home environm	nent
15. Disinfectants	
	,
Selected Crop: 7.2.1.2: Cut flowers	
V OK X Cancel	

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'

Projects	Run Help	Assessment Report	Show Graphs	? Help 🖉 Exit					ange les ≠ k∂ Sele
wse Assess	ments								ाउँ Editin
elected ID	Caption	Description	Results	Substance	Crop	CreationDate	Modificatio		-
								\mathbf{O}	
								õ	
Select all t Assessment Caption:	Deselect all Ints Uutput options Status ase 1_SB_GW_A1	Continue multiple runs on error	r Crop	p: Cut flowers			•	6	

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 $\sqrt{\prime}$ 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 ' $\sqrt{}'$ button

Nr.	ApplicationType /	Application Date	Dosage	Application parameter	6
1	To the crop canopy	15-Mar	0.06	0.5	
2	To the crop canopy	30-Mar	0.06	0.5	6
3	To the crop canopy	15-Sep	0.075	0.5	
4	To the crop canopy	30-Sep	0.075	0.5	11
				40)	
		3	5)	40)	

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:

Informati	on 💦
0	For Soilbound-groundwater assessments graphs are not made. Consequently the output tab is not applicable
	OK

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

Projects	Calculate	Assessment Report	Show Gra	ins	Help			
rowse Assessm	nents		1.4	Meet				
Selected ID	Caption	Description	Res	ults Subs	tance	Crop	CreationDate	Modificatio
6	Case1_SP_CW_41	Case1_SB_GW_A1	Fals	e PaT1	- PaT1_Parent_GEM-course	Cut flowers	24/01/2016	24/01/2016
		`						Þ
Select all	Deselect all	Continue multiple runs on	error					•
Select all	Deselect all	Continue multiple runs on	error					,
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Select all lit Assessment Assessmert Ou	Deselect all ts ts tput options Status LSB_GW_A1	Continue multiple runs on	error	Crop:	Cut flowers			, ,
Select all lit Assessmen t Assessment Ou c 44) Description: 100	Deselect all	Comments	error	Crop: Substance:	Cut flowers	PaT1_Parer	it GEM-course	
Select all lit Asses sment Assessmert Ou c 44) Description: ca	Deselect all ts htput options Status LSB_GW_A1 se1_SB_GW_A1	Comments	error	Crop: Substance:	Cut flowers	PaT1_Parer	it_GEM-course	+ 686
Select all lit Assessment Assessment Ou c 44) Description: co Manage appli	Deselect all ts htput options Status LSB_GW_A1 set_SB_GW_A1	Comments 45)		Crop: Substance:	Cut flowers PaT1 Mitigation	PaT1_Parer	it_GEM-course	, , , , , , , , , , , , , , , , , , ,
Select all Select all Select all Sel	Deselect all ts tput options Status LSB_GW_A1 set_SB_GW_A1 ication with regard to d val between application	I ⊂ Continue multiple runs on Comments 45) ischarge? and discharge [d] :		Crop: Substance:	Cut flowers PaT1 Mitigation	PaT1_Parer	it_GEM-course	

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.

Projects	Calculate	Assessment Report	Show Graphs	? Help 🖉 Exit				
owse Assessment								
selected ID Cap	ion	Descripticn	Result	s Substance	Crop	CreationDate	Modificatio	6
es 6 Case	1_S8_GW_A1	47)	True	PaIT1-PaIT1_Parent_GEM-course	Cut flowers	08/02/2016	08/02/2016	00000
Select all De	select all	✓ Continue multiple runs o	n error				Þ	Ć
Select all De Select all De Assessment Output Selected for executio CreationDate: ModificationDate: Results:	select all options Status 1. 08/02/2016 08/02/2016 available	Continue multiple runs o	n error ErrorMessage:				•	Ć

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.....

^h percentile PEC groundwater M1T1
--

Would the substance be approved (groundwater water criterion = 0.1 μ g/L and criterion for groundwater water abstraction areas = 0.01 μ g/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. <u>Please proceed now with the soil-bound-surface water project of CASE 1.</u>

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
- \circ 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 ' $\sqrt{'}$ 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

Selected D Caption Description Results Substance Crop CreationDate Hodification 7 Case1_SB_SW_A1 Case1_SB_SW_A1	Projects	Calculate	Assessment	Report Show	Graphs	? Help 🛛 🔇 Exit			
Selected ID Caption Description Results Substance Crop CreationDate Modification 7 Case1_SB_SW_A1 Case1_SB_SW_A1	rowse Assess	nents		12.					
7 Case1_SB_SW_A1 Case1_SB_SW_A1 False PaT1-PaT1_Parent_GEM-course Cut flowers 25/01/2016 25/01/2016 *	Selected ID	Caption	Description	1	Results	Substance	Crop	CreationDate	Modificatio
 ✓	7	Case1_SB_SW_A1	Case1_SB_SW_A1		False	PaT1 - PaT1_Parent_GEM-course	Cut flowers	25/01/2016	25/01/2016
Output and the manufact fund on entrol dit Assessments Assessment Output needed for report Image: All needed for viewing graphical output with GUI Exposure TWA Image: TWA Soilless Target percentile:									
C Output needed for report All needed for viewing graphical output with GUI Exposure TWA WA Soilless Target percentile: 90 v	 Select all 	Deselect all	Continue multiple	runs on error					,
Exposure Soilless TWA Image: Target percentile: Image: Target percentile: Image: Soilless	Select all	Deselect all status	Continue multiple	runs on error	ecting the	maximum concentration			,
	Select all Jit Assessment Assessment C Output ne (All needed	Deselect all	Continue multiple	Time window for sel	ecting the	maximum concentration			,

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.

I Proje	cts		Assessment Report	first snow Graph				
owse As	sessi	ments		-				
Selected	ID	Caption /	Descriptic n	Resu	Its Substance	Crop	CreationDate	Modific: ^
	7	Case1_SB_SW_A1	Cas	70)	PaT1 - PaT1_Parent_GEM-course	Cut flowers	25/01/2016	27/01/20
	20	Case1_SB_SW_A10	^{Cas} 69)	70)	PaT1 - PaT1_Parent_GEM-course	Cut flowers	25/01/2016	27/01/20
'es	21	Case1_SB_SW_A11	Cas		PaT1 - PaT1_Parent_GEM-course	Cut flowers	25/01/2016	27/01/20
'es	22	Case1_SB_SW_A12	Case1_SB_SW_A12	False	PaT1 - PaT1_Parent_GEM-course	Cut flowers	25/01/2016	27/01/20
'es	25	Case1_SB_SW_A13	Case1_SB_SW_A13	False	PaT1 - PaT1_Parent_GEM-course	Cut flowers	27/01/2016	27/01/20
'es	26	Case1_SB_SW_A14	Case1_SB_SW_A14	False	PaT1 - PaT1_Parent_GEM-course	Cut flowers	27/01/2016	27/01/20
'es	27	Case1_SB_SW_A15	Case1_SB_SW_A15	False	PaT1 - PaT1_Parent_GEM-course	Cut flowers	27/01/2016	27/01/20
'es	28	Case1_SB_SW_A16	Case1_SB_SW_A16	False	PaT1 - PaT1_Parent_GEM-course	Cut flowers	27/01/2016	27/01/20
'es	29	Case1_SB_SW_A17	Case1_SB_SW_A17	False	PaT1 - PaT1_Parent_GEM-course	Cut flowers	27/01/2016	27/01/20
'es	30	Case1_SB_SW_A18	Case1_SB_SW_A18	False	PaT1 - PaT1_Parent_GEM-course	Cut flowers	27/01/2016	27/01/20
'es	12	Case1_SB_SW_A2	Case1_SB_SW_A2	False	PaT1 - PaT1_Parent_GEM-course	Cut flowers	25/01/2016	27/01/20
'es	13	Case1_SB_SW_A3	Case1_SB_SW_A3	False	PaT1 - PaT1_Parent_GEM-course	Cut flowers	25/01/2016	27/01/20
'es	14	Case1 SB SW A4	Case1 SB SW A4	False	PaT1 - PaT1 Parent GEM-course	Cut flowers	25/01/2016	27/01/20
Select a	1	Deselect all	Continue multiple runs o	n error				
lit Assess Assessmer	t 0	utput options Status	Comments					
Selected f	or ex	ecution: Г		ErrorMessage:				
CreationD	ate:	25/01/2016	y					
Modificatio	nDat	e: 27/01/2016						
Results:		available						
				1				

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 μ g/L (L(E)C50 invertebrates) times an assessment factor of 0.01. The corresponding Regulatory Acceptable Concentration for the metabolite is 1100 μ g/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.

owse Projects				
D Caption	Description	CultivationType	CreationDate	ModificationDate
1 ExProject1	Example Project 1 soilless culti	Soilless - surface water	22/01/2016 10:13:33	22/01/2016 10:13:33
2 ExProject2	Example project 2 soil-bound-s	Soil-bound - surface water	22/01/2016 10:13:33	22/01/2016 10:13:33
3 ExProject3	Example project 3 soil-bound -	Soil-bound - ground water	22/01/2016 10:13:33	22/01/2016 10:13:33
5 Case1_SBSW	Case 1 Soilbound Surface wat	Soil-bound - surface water	24/01/2016 14:49:33	24/01/2016 14:50:05
6 Case1_SBGW	Case 1 Soilbound Groundwate	Soil-bound - ground water	24/01/2016 14:50:14	24/01/2016 14:50:24
7 Case2 SLSW	Case2 Soilless Surface water 2	Soilless - surface water	25/01/2016 15:30:38	25/01/2016 15:31:14
				5)
t Projects eneral Comments Case2	4) SLSW) CreationDate:	25/01/2016	5)
t Projects eneral Comments Caption: Case 2 Description: Case 2	4) SLSW Solless Surface water 2015-2017 filt	CreationDate:	25/01/2016	5)

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 ' $\sqrt{'}$ 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)

Edit View	Kun neip	a to a second second	1	1.	1	1				
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owse Assess	sments									
elected ID) Caption	Description		Results Su	ibstance	Cro	p	CreationDate	Modificatic	6
8	Case2_SL_SW_A1	Case2_SL_SW_A1		False		Cut	flowers	25/01/2016	25/01/2016	1
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Select all	Deselect all	Continue multiple ru	uns on error				9)		ł	
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Select all it Assessme Assessment (Deselect all ents Output options Status	Continue multiple ru	uns on error				9)		,	
Select all it Assessment (Cantion: 0	Deselect all ents Output options Status Case2 SI SW A1	Continue multiple ru	uns on error	Cropy	Cut flowers		9)		,	
Select all it Assessment d Caption: 0	Deselect all ents Output options Status Case2_SL_SW_A1	Continue multiple ru	uns on error	Crop:	Cut flowers		9)		,	
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Select all it Assessment of Caption: of Description: of	Deselect all ents Output options Status Case2_SL_SW_A1 Case2_SL_SW_A1	Continue multiple ru	uns on error	Crop: Substan	Cut flowers EXGE0 EXGE0	(incomplete) (incomplete)	9) GEM default valu GEM default valu	es for sol-bound es for sol-bound s	,	
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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:

×	Error	X
You have to save the changes before you can continue. Do you want to continue and save changes?	S S	ubstance should be selected.
<u>Yes</u> Cancel		ОК
	You have to save the changes before you can continue. Do you want to continue and save changes?	You have to save the changes before you can continue. Do you want to continue and save changes?

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.

Project	ts	Calculate	I Assessment Report	Show Gra	aphs					
~										
owse Ass	essm	ents	1	1				1		_
selected	ID	Caption	Description	Re	esults	Substance	Crop	CreationDate	Modificatio	(1
	5	F1_A1		Fal	lse	EXGE1 - GEM example substance for so	Cut flowers	26/11/2015	26/11/2015	Z
										11
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Select all	ment	Deselect all s	Continue multiple runs on er	error					Þ	
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Select all iit Assessi Assessment Caption: Description		Deselect all s s put options Status A1	Comments	error	Crop:	: Cut flowers	GEM examp	le substance for soil-b	,	
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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 ' \checkmark ' button

1.05716					2	-+)	
rowse S	ubstances						
ocked	SubstanceCode N	ame		CreationDate		LastMo	odified
9	EXGE0 G	EM default values for soil-bou	ind SW and soilless	18/01/2016 15:13:5	8	18/01/2	2016 15:13:58
8	EXGE1 G	EM example substance for so	il-bound SW and soilless	13/11/2014 14:26:0	2	13/11/2	2014 14:26:02
9	EXSW3 F	OCUS surface water Example	_Sub_6	25/06/2015 09:16:0	9	25/06/2	2015 09:16:09
	COPY G	EM default values for soil-bou	ind SW and soilless_copy	25/01/2016 15:42:3	1	25/01/2	2016 15:42:31
	M1T1 M	1T1_Metabolite1T1_GEM-cou	rse	22/01/2016 16:33:1	9	1.0.)	16 14:26:43
8	EXGE2 e:	cample substance for soil-bou	and GW	13/11/2014 14:26:0	2	12)	14 14:26:02
	PaT1 Pa	aT1_Parent_GEM-course		22/01/2016 15:54:2	3	22/01/2	016 16:20:33
8	EXSW1 F	OCUS surface water Example	_Sub_A	25/06/2015 09:16:			15 09:16:09
8	EXSW0 F	DCUS surface water Default_	values	25/06/2015 09:16:	14	I)	15 09: 16:09
8	EXGE3 es	kample metabolite for soil-boi	und GW	13/11/2014 14:26:0	-		14 14:26:02
<u>A</u>	EXSW4	OCUS surface water Example	_Sub_6m_sw, soil metabolite from 6_sw	25/06/2015 09:16:0	9	25/06/2	2015 09:16:09
	M2T1 M	2T1_Metabolite2T1_GEM-cou	irse	24/01/2016 14:27:5	5	24/01/2	2016 14:30:54
8	EXSW2 F0	DCUS surface water Example	Sub H	25/06/2015 09:16:0	9	25/06/2	2015 09:16:09
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lit Subs General Substa	tance Sorption Transformation Crop anceCode:	processes			18	;)	
lit Subs General Substa Name:	tance Sorption Transformation Crop anceCode:	p processes COPY GEM default values	for soil-bound SW and soilless_copy		18	;)	
lit Subs General Substa Name: Molar 1	tance Sorption Transformation Crop anceCode: mass (g mol-1):	p processes COPY GEM default values <no given="" value=""></no>	for soil-bound SW and soilless_copy		18	;)	
lit Subs General Substa Name: Molar i Satura	tance Sorption Transformation Crop anceCode: mass (g mol-1): tted vapour pressure (Pa):	p processes COPY GEM default values ⊲no value given> ⊲no value given>	for soil-bound SW and soilless_copy () () Measured at (°C):	20	18	;)	
lit Subs General Substa Name: Molar I Satura Molar I	tance Sorption Transformation Crop anceCode: mass (g mol-1): ated vapour pressure (Pa): enthalpy of vaporisation (kJ mol-1)	COPY GEM default values <no given="" value=""> <no given="" value=""> i: 95</no></no>	for soll-bound SW and soilless_copy	20	18	;)	
lit Subs General Substa Name: Molar I Satura Molar I Solubil	tance Sorption Transformation Crop anceCode: mass (g mol-1): ted vapour pressure (Pa): enthalpy of vaporisation (kJ mol-1) ity in water (mg L-1):	P processes COPY GEM default values <no given="" value=""> <no given="" value=""> 95 <no given="" value=""></no></no></no>	for soil-bound SW and soilless_copy	20	18 Ф	;)	
it Subs General Substa Name: Molar (Satura Molar (Solubil Molar (tance Sorption Transformation Crop anceCode: mass (g mol-1): ted vapour pressure (Pa): enthalpy of vaporisation (kJ mol-1) ity in water (mg L-1): enthalpy of dissolution (kJ mol-1):	P processes COPY GEM default values <no given="" value=""> <no given="" value=""> 95 <no given="" value=""> 27</no></no></no>	for sol-bound SW and solless_copy (i) Measured at (°C): (i) Measured at (°C): (i) Measured at (°C): (i)	20	18 Ф	;)	
lit Subs General Substa Name: Molar (Satura Molar (Solubil Molar (Refere d-1):	tance Sorption Transformation Crop anceCode: mass (g mol-1): ated vapour pressure (Pa): enthalpy of vaporisation (kJ mol-1) ity in water (mg L-1): enthalpy of dissolution (kJ mol-1): ence diffusion coefficient in water	P processes COPY GEM default values (no value given> 95 (no value given> 27 4.3E-5	for soil-bound SW and soilless_copy (i) Measured at (°C): (i) Measured at (°C): (i) Reference temperature (°C): (i) Reference temperature (°C):	20	18 Ф	;)	
Jit Subs General Substa Name: Molar 1 Satura Molar 1 Solubil Molar 1 Refere d-1): Refere	tance Sorption Transformation Crop anceCode: mass (g mol-1): ated vapour pressure (Pa): enthalpy of vaporisation (kJ mol-1) ity in water (mg L-1): enthalpy of dissolution (kJ mol-1): ence diffusion coefficient in water in ence diffusion coefficient in air (m2	p processes COPY GEM default values <no given="" value=""> <no given="" value=""> <no given="" value=""> <no given="" value=""> 27 4.3E-5 d-1): 0.43</no></no></no></no>	for soil-bound SW and soilless_copy (i) Measured at (°C): (i) Measured at (°C): (i) Measured at (°C): (i) Reference temperature (°C)	20	18 •	;)	

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 ' $\checkmark \prime \prime$ button

- 18) Select substance **Pa1T2** in the Browse substances table and click the metabolite scheme button:
- 19) Select the <u>Recirculation water tab</u> 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 ' $\sqrt{'}$ button
- 24) Repeat steps 19-23 for adding M1T2 as metabolite in surface water (select the <u>Surface water tab</u> 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

Projec	ts	Calculate	Assessment Repo	ort 🛛 😿 Show	w Graphs	? Help 🖉 Exit			
OWSE ASS	essin								
selected	8 0	Caption	Case? SL SW A1		False	Substance	Cut fowers	25/01/2016	25/01/2016
Select all	nent	Deselect all s tput options Status	Continue multiple runs	on error					•
Select all Select all Iit Assession Assessment Caption:	nent Out	Deselect all s s tput options Status se2_SL_SW_A1	Continue multiple runs	on error 26)	Crop	p: Cut flowers			•
Select all lit Assessing Assessment Caption: Description	nent Out	Deselect all s tput options Status se2_SL_SW_A1 se2_SL_SW_A1	Continue multiple runs	on error 26)	Crop	p: Cut flowers stance: PAT2	PaT2_Paren	t_GEM-course	, , , ,

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 ' $\sqrt{}$ ' 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 ' $\sqrt{'}$ 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.

	Application	ons				
Valid	Nr./	Application type	Target Application Date	Dosage	SearchInterval	6
Yes	1	Spraying	15-Mar	0.144	7	C
Yes	2	Spraying	22-Mar	0.144	7	6
Yes	3	Spraying	29-Mar	0.144	7	
Yes	4	Spraying	06-Apr	0.144	7	6
dit App Applica	lications tion type ed apolic	e: Spraying	.			
dit App Applica Intende date: Dosage Accept applica	lications tion type ed applic [kg.ha- able char tion date	2: Spraying ation Apr ▼ / 1]: 0.144 nge in 2 +/- [d]: 7	• 6 •		40)	

inlications:	date (Applic Nr)	2000	2001	2002	2003	2004	2005	2006		Legend:	
pirculation	13-03	2000	2001	2002	2005	2001	A (1)	2000		Discharge	Day of discharge
First	14-03						V // (-)	-		Discharge	buy of discillinge
	15-03 (1)	1 V	1 V	100	1 V 1	1 V 1		1 V 1		I. I.	Minimal interval between
Prev	16-03						Discharge				application and discharge
Next	17-03						Personal Contractor			1 V 1	Application
HEAL	18-03	1									
Last	19-03				a.1.					×	No solution found
0.01404	20-03										
	21-03		1.1		Discharge	1.1	1	1.1		VA (*)	New application date
	22-03 (2)				1 V					1074-01-04	
(i)	23-03										
w	24-03										
	25-03										
	26-03			Discharge							
	27-03				🖌 A (3)						
	28-03	_		101		125	1.0				
	29-03 (3)	V	V .	V	1	V .	V	V.			
	30-03				Discharge						
	31-03										
	01-04										
	02-04										
	03-04	41									
	04-04							🖌 A (4)			
	05-04	Discharge	100	100	0.00	1.0	0.0			_	
	06-04 (4)		V.	V	V	V	V	6			(2)
	07-04							Discharge			42)
	08-04									L	
	09-04					x					
	10-04					Discharge					
	11-04		12								
	12-04								*		

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).

	reduction		111
Substance	Removal factor		6
M1T2	0.75		
Pa1T2	0.75		
		46)	
E dit end-of-pipe red Substance:	uction Pa1T2		48)

- 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 ' $\sqrt{}'$ 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

GEM	1.1.1
	Information
The	e removal fraction defines the reduction as fraction of the discharged mass.E.g. a removal fraction of 0.4 reduces the daily discharged mass to surface water with 40%.
	(Close)

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'

AEL	ts	Calculate	Assessment Re	eport 🛛 😿 Sho	ow Graphs	? Help 🛛 🔇 Exit			
rowse Ass	essment	,		1.4					
Selected	ID Cap	tion	Description		Results	Substance	Crop	CreationDate	Modificatio
	8 Case	2_SL_SW_A1	Case2_SL_SW_A1		False	PAT2 - PaT2_Parent_GEM-course	Cut flowers	25/01/2016	25/01/2016
 Select all dit Assess Assessmen 	De ments : Output	eselect all	Continue multiple	49)				E1)	•
	ut needed	for report iewing graphical o	utput with GUI	Time window for	selecting the	maximum concentration		51)	
© Outp Oll ne Exposure		Ø	50)	Target percentil	e: 50			•	

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 50^{th} or a 90^{th} 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 ' $\sqrt{'}$ button
- 59) Leave the TWA screen by clicking the 'Close' button

Defaults:				
Name	Duration [d]	Start Relevant Period	End Relevant Period	i i i
TWA7	7	01-Jan	31-Dec	
TWA21	21	01-Jan	31-Dec	
Additional (max 8 + 2):				
Name	Duration [d]	Start Relevant Period	End Relevant Period	6
TWA 14d	14	01-Mar	31-Oct	
			55) 59)	
			55) 59)	
			55) 59) 58)	

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.

owse Assessments		1				
ielected ID Caption	Description	Results Sul	ostance	Crop	CreationDate	Modificatio
8 Case2_SL_SW_A1	Case ² Cl. Cl. 11	65) PAT	2 - PaT2_Parent_GEM-course	Cut flowers	25/01/2016	25/01/2016
	64)	05)				
						•
Select all Deselect all 1	✓ Continue multiple runs on e	rror				ŀ
Select all Deselect all	✓ Continue multiple runs on e	rror				,
Select all Deselect all	✓ Continue multiple runs on e	rror				•
Select all Deselect all I	✓ Continue multiple runs on e	rror				•
Select all Deselect all F it Assessments ssessment Output options Status C	✓ Continue multiple runs on e Comments)	rror				Þ
Select all Deselect all I it Assessments ussessment Output options Status C	Continue multiple runs on e Comments	rror indow for selecting the maxi	num concentration			F
Select all Deselect all F it Assessments ssessment Output options Status C C Output needed for report	Continue multiple runs on e	rror	num concentration			,
Select all Deselect all F it Assessments ssessment Output options Status C C Output needed for report C Output needed for viewing graphical out	Continue multiple runs on e comments	rror indow for selecting the maximity $ 1 + 10000000000000000000000000000000000$	num concentration			,
Select all Deselect all F it Assessments ussessment Output options Status C C Output needed for report C Output needed for viewing graphical out	Continue multiple runs on e Comments Dut with GUI	rror indow for selecting the maximum $\sqrt{1}$ to Dec	num concentration			Þ
Select all Deselect all F it Assessments ussessment Output options Status C C Output needed for report C All needed for viewing graphical out Exposure	Continue multiple runs on e Comments Time w Jan Soilless	indow for selecting the maxim	hum concentration			b
Select all Deselect all I it Assessments Assessment Output options Status C C Output needed for report All needed for viewing graphical out Exposure TWA	Continue multiple runs on e comments put with GUI	rror indow for selecting the maxin Image: Image: Im				<u></u> ,
Select all Deselect all F it Assessments Assessment Output options Status C C Output needed for report (All needed for viewing graphical out Exposure TWA	Continue multiple runs on e Comments Comments Comments Comments Comments Comments Comments Continue Co	indow for selecting the maxim v / 1 v to Dec t percentile: 50				, , , , , , , , , , , , , , , , , , ,
Select all Deselect all F it Assessments Understand Status C C Output needed for report C Output needed for viewing graphical out Exposure TWA	Continue multiple runs on e Comments	rror indow for selecting the maxin $\mathbf{v} / 1 \mathbf{v}$ to Dec t percentile: 50	num concentration			F.

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

 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	, 411.82	L.kg ⁻¹	Measured at 20 °C
sediment and suspended solids (Kom)			
Reference concentration in liquid phase in soil/sediment/	1	mg.L ⁻¹	
suspended solids			
Freundlich exponent in soil/sediment/ suspended solids	0.98	-	
Saturated vapour pressure	4.E-6	Ра	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	µg.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	m² d ⁻¹	Measured at 20 °C
Reference diffusion coefficient in air	0.43	m² 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,	45.26	L.kg⁻¹	Measured at 20 °C
sediment and suspended solids (Kom)			
Reference concentration in liquid phase in soil/sediment/	1	mg.L⁻¹	
suspended solids			
Freundlich exponent in soil/sediment/ suspended solids	0.95	-	
Saturated vapour pressure	1.E-10	Ра	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	µg.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	m² d ⁻¹	Measured at 20 °C
Reference diffusion coefficient in air	0.43	m² d ⁻¹	Measured at 20 °C
Molar enthalpy of sorption	0	kJ mol ⁻¹	
Molar activation energy in soil	65.4	k1 mol ⁻¹	
	05.4	KJ IIIOI	
Molar activation energy in water	65.4	kJ mol ⁻¹	
Molar activation energy in water Molar activation energy in sediment	65.4 65.4	kJ mol ⁻¹ kJ mol ⁻¹	

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
Sep-Nov	2	15	To the crop canopy	0.075	0.5	first application on the 15th

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	0.8	d	Measured at 25 °C and
disinfection tank			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	Ра	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	µg.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	m² 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	1.2	d	Measured at 25 °C and
disinfection tank			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,	5124	L.kg ⁻¹	
sediment and suspended solids (Kom)			
Reference concentration in liquid phase in sediment/	1	mg.L⁻¹	
suspended solids			
Freundlich exponent in sediment/ suspended solids	0.9	-	
Saturated vapour pressure	1E-10	Ра	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	µg.L⁻¹	
assessment factor	100		0.01 times the L(E)C50
Defaults			
Defaults Property	value	unit	comment
Defaults Property Molar activation energy in greenhouse air	value 45	unit kJ mol ⁻¹	comment
Defaults Property Molar activation energy in greenhouse air Molar activation energy in recirculation water	value 45 65.4	unit kJ mol ⁻¹ kJ mol ⁻¹	comment
Defaults Property Molar activation energy in greenhouse air Molar activation energy in recirculation water Molar enthalpy of vaporisation	value 45 65.4 95	unit kJ mol ⁻¹ kJ mol ⁻¹ kJ mol ⁻¹	comment
Defaults Property Molar activation energy in greenhouse air Molar activation energy in recirculation water Molar enthalpy of vaporisation Molar enthalpy of dissolution	value 45 65.4 95 27	unit kJ mol ⁻¹ kJ mol ⁻¹ kJ mol ⁻¹ kJ mol ⁻¹	comment
Defaults Property Molar activation energy in greenhouse air Molar activation energy in recirculation water Molar enthalpy of vaporisation Molar enthalpy of dissolution Reference diffusion coefficient in water	value 45 65.4 95 27 4.3E-5	unit kJ mol ⁻¹ kJ mol ⁻¹ kJ mol ⁻¹ kJ mol ⁻¹ m ² d ⁻¹	comment Measured at 20 °C
Defaults Property Molar activation energy in greenhouse air Molar activation energy in recirculation water Molar enthalpy of vaporisation Molar enthalpy of dissolution Reference diffusion coefficient in water Reference diffusion coefficient in air	value 45 65.4 95 27 4.3E-5 0.43	unit kJ mol ⁻¹ kJ mol ⁻¹ kJ mol ⁻¹ kJ mol ⁻¹ m ² d ⁻¹ m ² d ⁻¹	comment Measured at 20 °C Measured at 20 °C
Defaults Property Molar activation energy in greenhouse air Molar activation energy in recirculation water Molar enthalpy of vaporisation Molar enthalpy of dissolution Reference diffusion coefficient in water Reference diffusion coefficient in air Molar activation energy in water	value 45 65.4 95 27 4.3E-5 0.43 65.4	unit kJ mol ⁻¹ kJ mol ⁻¹ kJ mol ⁻¹ kJ mol ⁻¹ m ² d ⁻¹ kJ mol ⁻¹	comment Measured at 20 °C Measured at 20 °C
Defaults Property Molar activation energy in greenhouse air Molar activation energy in recirculation water Molar enthalpy of vaporisation Molar enthalpy of dissolution Reference diffusion coefficient in water Reference diffusion coefficient in air Molar activation energy in water Molar activation energy in sediment	value 45 65.4 95 27 4.3E-5 0.43 65.4 65.4	unit kJ mol ⁻¹ kJ mol ⁻¹ kJ mol ⁻¹ kJ mol ⁻¹ m ² d ⁻¹ m ² d ⁻¹ kJ mol ⁻¹ kJ mol ⁻¹	comment Measured at 20 °C Measured at 20 °C

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 Gewasbeschermingsmiddelen" (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
Sep-Nov	2	15	To the crop canopy	0.075	0.5	first application on the 15th

Applications dates	90 th percentile PEC	90 th percentile PEC	
	groundwater Pa1T1 (ug/L)	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
Sep-Nov	2	15	To the crop canopy	0.075	0.5	first application on the 15th

Applications dates	90 th percentile PEC surface water Pa1T1 (ug/L)	90 th 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 μ g/L (L(E)C50 invertebrates) times an assessment factor of 0.01. The corresponding Regulatory Acceptable Concentration for the metabolite is 1100 μ g/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	50 th percentile PEC surface water Pa1T2 (ug/L)	50 th 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 μ g/L (L(E)C50 invertebrates) times an assessment factor of 0.01. The corresponding Regulatory Acceptable Concentration for the Metabolite is 44 μ g/L (L(E)C50 fish) times an assessment factor of 0.01.