



Wettelijke Onderzoekstaken Natuur & Milieu

SPIN Manual 1.1

User's Guide version 1, for use with FOCUS_SWASH 4.2

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M.S. ter Horst, G. Fait & J.A. te Roller

SPIN 1.1 Manual

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Abstract

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This manual addresses the main functionalities of the Substance Plug IN tool, SPIN version 1.1, which is released together with FOCUS_SWASH 4.2 and FOCUS_TOXSWA 4.4.2. SPIN is basically a database that stores all substance properties relevant to the listed pesticide fate software. New substances can be added to the database by copying an existing substance or by creating a new substance. The database can also be copied and exchanged between (advanced) users, whereas substances can also be exported and imported. SPIN can be run in two different modes, either standalone, 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 are accessible. SPIN has been developed such that all new releases of SPIN can communicate with earlier released host-applications.

Key words: Manual, pesticide properties, pesticide registration, software tool

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Preface

In 2009, the first ideas were launched to develop a central database that could be connected to all of our Pesticide Fate models. A few month after, a prototype of SPIN (Substance Plug IN) was built by Daniel van Kraalingen. Further refining and improving resulted in the first release of SPIN in 2010 coupled to the host-application TOPRICE, an exposure assessment tool for pesticides used on rice in China.

Because SPIN was (and still is) intended to become the spider in the web of our software tools we had occasionally heated internal discussions and disputes about the functionalities of SPIN. Looking back on the development process, we may conclude that these discussions where worthwhile and really improved the structure and user-friendliness of SPIN. At present, we are proud to release SPIN together with FOCUS_SWASH and FOCUS_TOXSWA.

This manual belongs to the first SPIN release as a supporting tool for the European pesticide risk evaluation. By developing SPIN, a new step has been taken toward more efficient and user friendly pesticide risk models. We hope that our effort improves the support of occasional users, but also of frequent and advanced users of our fate models.

Louise Wipfler (SPIN release manager)

Wageningen, 30 August 2013.

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Summary

This manual belongs to the Substance Plug IN tool, SPIN 1.1., which is released together with FOCUS_SWASH 4.2 and FOCUS_TOXSWA 4.4.2. The manual addresses the main functionalities of SPIN.

SPIN is basically a database that stores all substance properties that are relevant to all exposure assessment tools that are listed. New substances can be added to the database by copying an existing substance or by creating a new substance. The database can also be copied and exchanged between (advanced) users, whereas substances can also be exported and imported from one user to the other.

SPIN can be run in two different modes. Either standalone, 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 are accessible.

Substance properties can be entered and saved on the different tabs in the Edit Substance part of the main window. For each property an entry field is provided as well as a short description with units. After a property has been entered by the user, SPIN checks whether the entered value falls within a defined range. Information buttons provide additional background information.

Tabs allow for entering various property values. They are organized according to the processes that they address, i.e. 'General', 'Sorption', 'Transformation' and 'Crop processes'. At a lower level, each sub-tab addresses specific compartments i.e. soil, surface water, sediment and substrate (for greenhouse applications).

SPIN has been developed such that all new releases of SPIN can communicate with earlier released host-applications.

An import-export option in SPIN enables easy exchange of data, especially for frequent users and users collaborating with others.

1 Introduction

This manual belongs to the software tool SPIN 1.1. SPIN 1.1. has been released together with FOCUS_SWASH 4.2 and FOCUS_TOXSWA 4.4.2.

SPIN (Substance Plug IN) enables the storage of pesticide properties in a common database that can be accessed by different pesticide fate models from Alterra Wageningen UR. SPIN can also be used as a stand-alone application. SPIN can be downloaded from the EFSA website. Alterra intends to combine SPIN with all future pesticide fate software releases of Alterra.

This manual addresses the main functionalities of SPIN. Also, guidance on the use of SPIN is provided specific in relation to the host-applications FOCUS_SWASH 4.2 and FOCUS_TOXSWA 4.4.2 (Faith *et al.* (2013) and Beltman *et al.* (in prep). The examples and figures shown are related to FOCUS_SWASH 4.2.

Background

Pesticide fate software addresses a range of protection goals, i.e. FOCUS_PEARL4.4.4 is specific for pesticide leaching to groundwater and FOCUS_SWASH 4.2 is developed for the exposure calculation of aquatic ecosystems. For each of these models/tools, substance specific characteristics have to be entered to calculate the Relevant Environmental Concentrations. To assess the risk related to different protection goals, an assessor often has to use multiple fate models. For these users, entering substance properties can be time consuming, whereas often the same substance properties are applicable to the different models. SPIN has been developed to simplify the work of the risk assessor. SPIN makes it easier to manage and store substance properties by making them accessible for multiple pesticide fate models.

SPIN philosophy

SPIN is basically a database that stores all substance properties that are relevant to all pesticide models that are listed. The user-interface facilitates access to the database and the interaction with the user. Each substance has a unique code, a name and a short description. New substances can be added easily to the database by copying an existing substance or by creating a new substance. The database can also be copied and exchanged between (advanced) users, whereas substances can also be exported and imported from one user to the other. SPIN automatically creates a new database, when it detects no existing database e.g. when the old database has been archived or removed.

SPIN is linked to exposure assessment tools, which are referred to as host-applications (now FOCUS_SWASH 4.2 and FOCUS_TOXSWA 4.4.2).

SPIN can be run in two different modes. Either standalone, 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 are accessible.

Substance properties can be entered and saved on the different tabs in the Edit Substance part of the main window. For each property an entry field is provided with as well as a short description with units and an entry field. After a property has been entered by the user, SPIN checks whether the entered value falls within a defined range. Information buttons, at the right side of the entry field, provide background information, including ranges.

The tabs are organized according to the processes that they address, i.e. 'general', 'sorption', 'transformation' and 'crop processes'. At a lower level, each sub-tab addresses specific compartments i.e. soil, surface water, sediment and substrate (for greenhouse applications).

Because each host-applications may require a different default value for the same substance property, default values are not filled in automatically for newly created substances. To facilitate easy creation of new substances, example substances are provided for each host application, which can be copied and modified.

SPIN has been developed such that all new releases of SPIN can communicate with earlier released host-applications.

An import-export option in SPIN enables easy exchange of data, especially for frequent users.

2 Starting SPIN

2.1 Installation

SPIN is a software application that consists of a database and some DLL software to be used by either the stand-alone SPIN, or one of the host pesticide fate applications. During the installation procedure the software is placed by default under the current program files directory ("C:/Program Files/Pesticidemodels/SPIN" for 32 bit Windows systems, and "C:/Program Files (x86)/Pesticidemodels/SPIN" for 64 bit Windows systems). The user can change this directory, but is advised to not change it. The default directory for the database can also be changed by the user. It is mandatory to choose a directory on a disk that is local to the PC, such as the C drive. SPIN automatically creates a new database, when it detects no database e.g. when the old database has been archived or removed.

In case you want to upgrade an existing installation, you may uninstall SPIN and reinstall the newer version. This, however, is not really necessary. You can simply install the newer version of SPIN. The installation procedure is made such that an old database file is never deleted by uninstalling and never overwritten by reinstalling. In other words, the substance data are safeguarded. In cases where the newer version of SPIN requires a database update it will do so and inform the user through a progress windows. After upgrading, SPIN should work as expected.

The installation procedure in case of multiple users for one PC or laptop is explained in Appendix 1.

2.2 Starting up

After clicking on the SPIN icon (stand-alone) or the 'edit substance' button of a host-application, the main window is opened (see Figure 1). The caption at the top shows the version number of SPIN and the host-applications which SPIN is assuming. There is a menu bar below the caption text. The main window shows also the Browse substances section, including the clickable buttons to the right and the Edit substance section. In the Browse section, substances are selected which can be edited in the Edit section below.

The grid with substances will have some (example) substances which are locked for changes (and deleting). These substances are shown with a lock symbol in the first column of the grid. When such a substance is selected, none of the property fields will be enabled for editing.

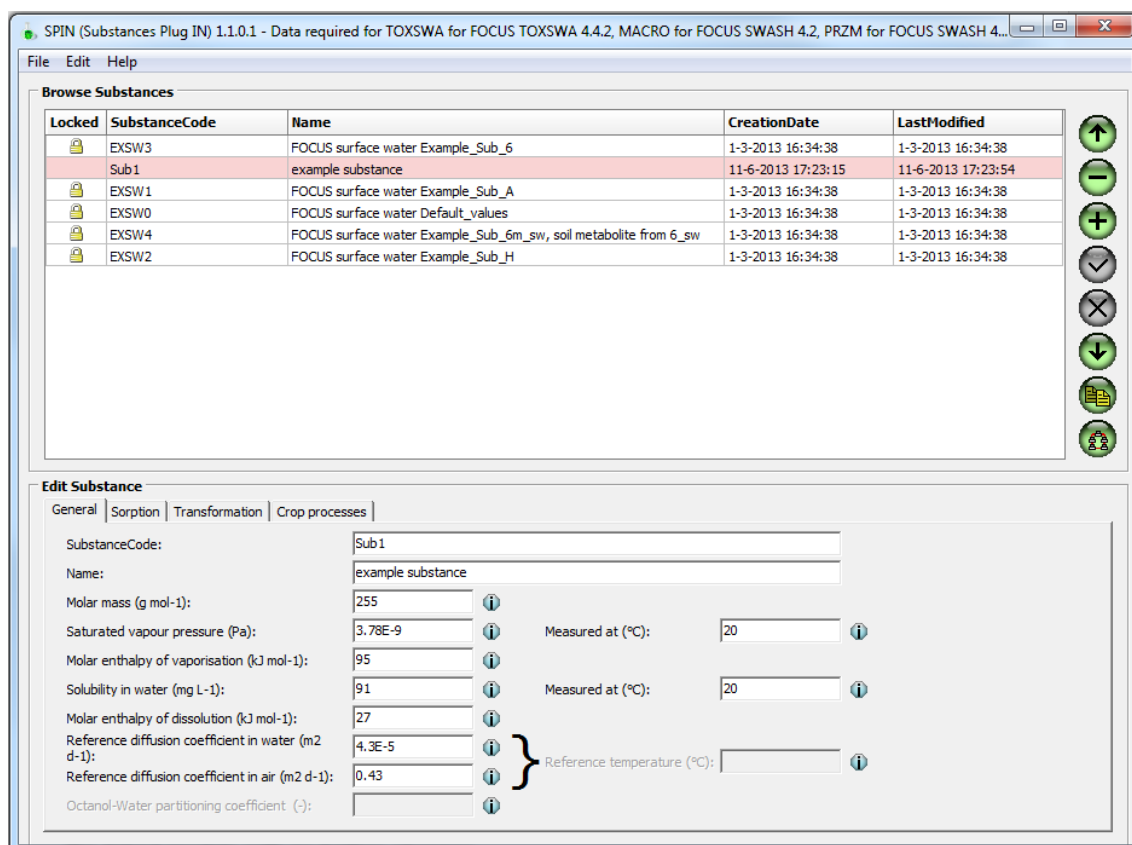


Figure 1: SPIN main window

2.3 Menu bar

Through the menu bar it is possible to select three options:

- 1) the **File** menu option allows the user to import and export substances and to close the application. Importing and exporting of substances is explained in Chapter 5.
- 2) the **Help** menu option allows the user to find detailed information about SPIN, such as the User Interface version, the database version and the path to the database. Through the menu 'help' one can access the model notes and a link to this manual.
- 3) the **Edit** menu option. The 'Edit' option is only shown in case SPIN is opened as a stand-alone application. The 'Edit' option allows the user to choose one (or more) model(s) and to enter only the properties required by the chosen model(s).

If SPIN is started as a standalone application and none of the models is selected, the user may enter all the substance properties listed in SPIN.

If SPIN is started through one of the host-applications, SPIN will automatically show the substance parameter specific for that host-application written in black. The other substance properties are disabled and drawn in grey.

2.4 Management of stored substances

In the 'Browse substances' section all substances saved in the database are shown (Figure 1). The substances are identified by a unique code and a name. Furthermore, the creation and the last modified dates are shown. After installation, a number of example substances, specific for each host-application, are present in the SPIN database.

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



create 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

The buttons are displayed in green when their function is allowed or in grey when their function is not allowed. The creation of metabolites (last button) is explained in Chapter 4.

3 Create or edit substances

3.1 Creating a substance

Creating and copying substances can be done by using the action buttons on the right side of the main window (see Section 2.2.3). When entering a new substance or when copying an existing substance, the substance code and the name of the substance have to be specified and to be unique. The substance code cannot exceed the five characters (for historical reasons), otherwise an error message will appear.

3.2 Editing a substance

3.2.1 The 'Edit substances' section

Within the 'Edit substances' section, it is possible to modify all the properties of a substance (Figure 2).

The 'Edit Substance' window has four tabs: General, Sorption, Transformation, and Crop processes. The 'General' tab is active. It contains the following fields:

SubstanceCode:	Sub1
Name:	example substance
Molar mass (g mol ⁻¹):	255
Saturated vapour pressure (Pa):	3.78E-9
Molar enthalpy of vaporisation (kJ mol ⁻¹):	95
Solubility in water (mg L ⁻¹):	91
Molar enthalpy of dissolution (kJ mol ⁻¹):	27
Reference diffusion coefficient in water (m ² d ⁻¹):	4.3E-5
Reference diffusion coefficient in air (m ² d ⁻¹):	0.43
Octanol-Water partitioning coefficient (-):	

On the right side, there are two 'Measured at (°C):' fields, both set to 20. A bracket groups the diffusion coefficient fields with a 'Reference temperature (°C):' field.

Figure 2: The 'Edit Substance' section. This section contains four main tabs that each address a fate process, i.e. General, Sorption, Transformation and Crop processes.

Next to each entry field there is an information button, which, when clicked, shows information about the substance property such as unit, description, minimum and maximum values, the model for which the parameter is required, and the internal code. An example is shown in Figure 3 for the substance property 'Molar mass'.

The 'Information on "Molar mass"' window displays the following details:

Unit:	g mol ⁻¹
Description:	Molar mass
Minimum value:	10
Maximum value:	10000
Default value:	It is SPIN policy to not provide default values
Required for:	TOXSWA for FOCUS TOXSWA 4.4.2 and higher, MACRO for FOCUS SWASH 4.2 and higher, TOXSWA for DRAINBOW and higher, PEARL for DRAINBOW and higher, PRZM for FOCUS SWASH 4.2 and higher, TOXSWA for GEM and higher, Substrate model for GEM and higher
Internal name:	MolMass (id=7)

Figure 3: Example information window for the input parameter 'Molar mass'.

The 'Edit substance' form is divided in four tabs: General, Sorption, Transformation, and Crop processes.

3.2.2 General tab

The properties listed in the general tab are (see Figure 2):

- the molar mass (g mol^{-1});
- the saturated vapour pressure (Pa) and the reference temperature at which vapour pressure was measured ($^{\circ}\text{C}$);
- the molar enthalpy of vaporisation (kJ mol^{-1});
- the solubility in water (mg L^{-1}) and the reference temperature at which solubility was measured ($^{\circ}\text{C}$);
- the molar enthalpy of dissolution (kJ mol^{-1});
- the reference diffusion coefficient in water ($\text{m}^2 \text{d}^{-1}$) and in air ($\text{m}^2 \text{d}^{-1}$) and the reference temperature at which these were measured ($^{\circ}\text{C}$);
- the octanol-water partition coefficient (-).

3.2.3 Sorption tab

Under the tab 'Sorption' (Figure 4), there are four sub-tabs: Soil, Surface water, Sediment and Substrate. The 'Substrate' tab (greenhouse) is not discussed in this manual, since it is not relevant for FOCUS_SWASH and FOCUS_TOXSWA.

The sorption in **Soil** tab is divided in two parts:

- the **Equilibrium sorption** part enables to choose among three different options for sorption in soil: Kf user defined, Kom pH-dependent, and Kom pH-independent (Figure 5). When the option Kf user defined or Kom pH-independent is chosen, the corresponding Kf (kg L^{-1}) or Kom (kg L^{-1}) values have to be entered. When the option Kom pH-independent is selected, then the Kom acid (kg L^{-1}), Kom base (kg L^{-1}), the pH correction and the pKa values have to be entered in SPIN. Furthermore, the temperature at which values were measured ($^{\circ}\text{C}$), the reference concentration in the liquid phase (mg L^{-1}), the molar enthalpy of sorption (kJ mol^{-1}) and the Freundlich sorption exponent can be provided (only in the stand-alone version; not needed for FOCUS_SWASH and FOCUS_TOXSWA).

When only the Koc value is available for a certain substance, the user can click on the magic wand icon, and the "Koc to Kom converter" window will be opened (Figure 6). Here the user can enter the Koc value and after clicking on OK the corresponding Kom will be automatically shown.

- the **Non-equilibrium sorption** part enables to enter the desorption rate coefficient (d^{-1}) and the factor relating Freundlich coefficient for non-equilibrium sorption and equilibrium sorption. This part is not relevant to FOCUS_SWASH and FOCUS_TOXSWA.

The screenshot shows the 'Edit Substance' window with the 'Sorption' tab selected. Under the 'Soil' sub-tab, the 'Equilibrium sorption' section is active. The 'Option' dropdown is set to 'Kom, pH-independent'. The 'Kom (L kg⁻¹)' field contains the value '38.28'. Below this, there are fields for 'Measured at (°C)', 'Reference concentration in liquid phase (mg L⁻¹)', 'Molar enthalpy of sorption (kJ mol⁻¹)', and 'Freundlich sorption exponent (-)' with a value of '1'. The 'Non-equilibrium sorption' section is also visible, with fields for 'Desorption rate coefficient (d⁻¹)' and 'Factor relating Freundlich coefficient for non-equilibrium sorption and equilibrium sorption (-)'.

Figure 4: Sorption in soil tab. This tab addresses equilibrium sorption and non-equilibrium sorption.

Edit Substance

General | Sorption | Transformation | Crop processes

Soil | Surface water | Sediment | Substrate

Equilibrium sorption

Option: Kom, pH-independent

Measured at (°C): <no value given>

Reference concentration: Kom, pH-independent

Molar enthalpy of sorption (kJ mol⁻¹):

Freundlich sorption exponent (-): 1

Kom, pH-independent

Kom (L kg⁻¹): 38.28

Non-equilibrium sorption

Desorption rate coefficient (d⁻¹):

Factor relating Freundlich coefficient for non-equilibrium sorption and equilibrium sorption (-):

Figure 5: Options for equilibrium sorption in soil.

Koc to Kom converter

Formulas used

Koc (L.kg⁻¹) = 1.724 * Kom (L.kg⁻¹)

Kom (L.kg⁻¹) = Koc (L.kg⁻¹) / 1.724

Current

Kom (L.kg⁻¹): 38.28

Converted to Koc (L.kg⁻¹): 65.99472

New

Converted to Kom (L.kg⁻¹): 38.28

Enter Koc value (L.kg⁻¹) -----> 65.99472

OK Cancel

Figure 6: The Koc to Kom converter window.

The sorption in **Surface water** tab is divided in two parts (Figure 7):

- the **Equilibrium sorption in suspended solids** part where it is possible to enter the Kom value (L kg⁻¹) in suspended solids, the Freundlich sorption exponent and the reference concentration (mg L⁻¹). Also here, clicking on the magic wand symbol opens the “Koc to Kom converter” tool (Figure 6).
- the **Equilibrium sorption in macrophytes** part where the coefficient for linear sorption on macrophytes (L kg⁻¹) can be set.

Edit Substance

General | Sorption | Transformation | Crop processes

Soil | Surface water | Sediment | Substrate

Equilibrium sorption in suspended solids

Kom (L.kg⁻¹): 38.28

Freundlich sorption exponent (-): 1

Reference concentration (mg L⁻¹): 1

Equilibrium sorption in macrophytes

Coefficient for linear sorption on macrophytes (L.kg⁻¹): 0

Figure 7: Sorption in surface water tab.

In the **Sorption in sediment** tab the K_{om} ($L\ kg^{-1}$) in sediment, the Freundlich sorption exponent and the reference concentration ($mg\ L^{-1}$) values can be entered (Figure 8). Also here, clicking on the magic wand symbol opens the “Koc to K_{om} converter” tool (Figure 6).

Figure 8: Sorption in sediment tab.

3.2.4 Transformation tab

Under the tab Transformation (Figure 9) there are five sub-tabs: Soil-aerobic, Soil-anaerobic, Surface water, Sediment and Other. The ‘Soil-anaerobic’ and the ‘Other’ tabs are not discussed here, since these are not relevant to FOCUS_SWASH and FOCUS_TOXSWA.

In the **Soil-aerobic** transformation tab it is possible to enter the following properties:

- the soil half-life (d) and the temperature at which was measured ($^{\circ}C$);
- a check box for the exponent for moisture conditions ($pF=2$ or wetter);
- exponent for the effect of liquid (-);
- the molar activation energy ($kJ\ mol^{-1}$);
- a check box to use the bi-phasic option;
- the moisture content as measured in transformation study (%);
- the option for moisture content in transformation study (relative to soil or relative to field capacity);
- the Q_{10} factor for the effect of temperature on transformation;
- the pF at which DT_{50} is measured ($\log(cm)$);
- the effect of temperature (K^{-1}).

Figure 9: The soil-aerobic transformation tab.

The option for moisture conditions ($pF=2$ or wetter) can be checked. Then, the value of liquid content in incubation experiment ($kg\ kg^{-1}$) has to be entered. This option is not relevant to FOCUS_SWASH or FOCUS_TOXSWA.

The option for biphasic transformation can be checked. Then, the value of half-life of second phase transformation (d) has to be entered as well as the days after initial application bi-phasic half-life begins (d).

The **surface water** transformation tab is divided in two parts (Figure 10):

- the **Water layer of water body** where it is possible to enter the water half-life (d) and the temperature at which was measured ($^{\circ}\text{C}$), and the molar activation energy (kJ mol^{-1});
- the **Water layer of paddy field** where only parameter is the half-life in a paddy layer (d). This option is not relevant to FOCUS_SWASH or FOCUS_TOXSWA.

The screenshot shows the 'Edit Substance' window with the 'Transformation' tab selected. Under the 'Surface water' sub-tab, there are two sections. The first section, 'Water layer of water body', contains three input fields: 'Half-life (d):' with the value 24, 'Measured at ($^{\circ}\text{C}$):' with the value 20, and 'Molar activation energy (kJ mol^{-1}):' with the value 65.4. The second section, 'Water layer of paddy field', contains one input field: 'Half-life in paddy layer (d):' which is currently empty. Information icons are present next to each input field.

Figure 10: The surface water transformation tab.

In the **Sediment transformation** tab, values can be entered for the sediment half-life (d) and the temperature at which was measured ($^{\circ}\text{C}$), and the molar activation energy (kJ mol^{-1}) (Figure 11).

The screenshot shows the 'Edit Substance' window with the 'Transformation' tab selected. Under the 'Sediment' sub-tab, there is one section: 'Sediment of waterbody'. It contains three input fields: 'Half-life (d):' with the value 24, 'Measured at ($^{\circ}\text{C}$):' with the value 20, and 'Molar activation energy (kJ mol^{-1}):' with the value 65.4. Information icons are present next to each input field.

Figure 11: The sediment transformation tab.

3.2.5 Crop processes tab

The crop processes tab is divided into two parts (Figure 12):

- In the **Canopy** part the wash-off factor (m^{-1}) can be entered. A drop down menu allows to choose among three options for canopy process: Lumped, Specified and Calculated. When the option 'Lumped' is selected, then only the half-life at crop surface (d) is required. When the option 'Specified' is selected, the half-lives for penetration, transformation and volatilization (d) have to be specified. When the option 'Calculated' is chosen, then the half-lives (d) due to penetration and transformation have to be entered. For FOCUS_SWASH and FOCUS_TOXSWA only the Lumped option can be chosen.
- In the **Plant root** part the coefficient for uptake by the plant (TSCF) has to be specified.

Edit Substance

General | Sorption | Transformation | Crop processes

Canopy

Wash-off factor (m-1): ⓘ

Canopy process option: ⓘ

Lumped

Half-life on crop canopy (d): ⓘ

Plant root

Coefficient for uptake by plant (TSCF) (-): ⓘ

Figure 12: Crop processes tab.

4 Create metabolite schemes

To link a metabolite to a parent substance, first the metabolite substance has to be created (see Chapter 3). Then, the parent substance should be selected, and the metabolite window opens by clicking on the open metabolites box symbol , as shown in Figure 13.

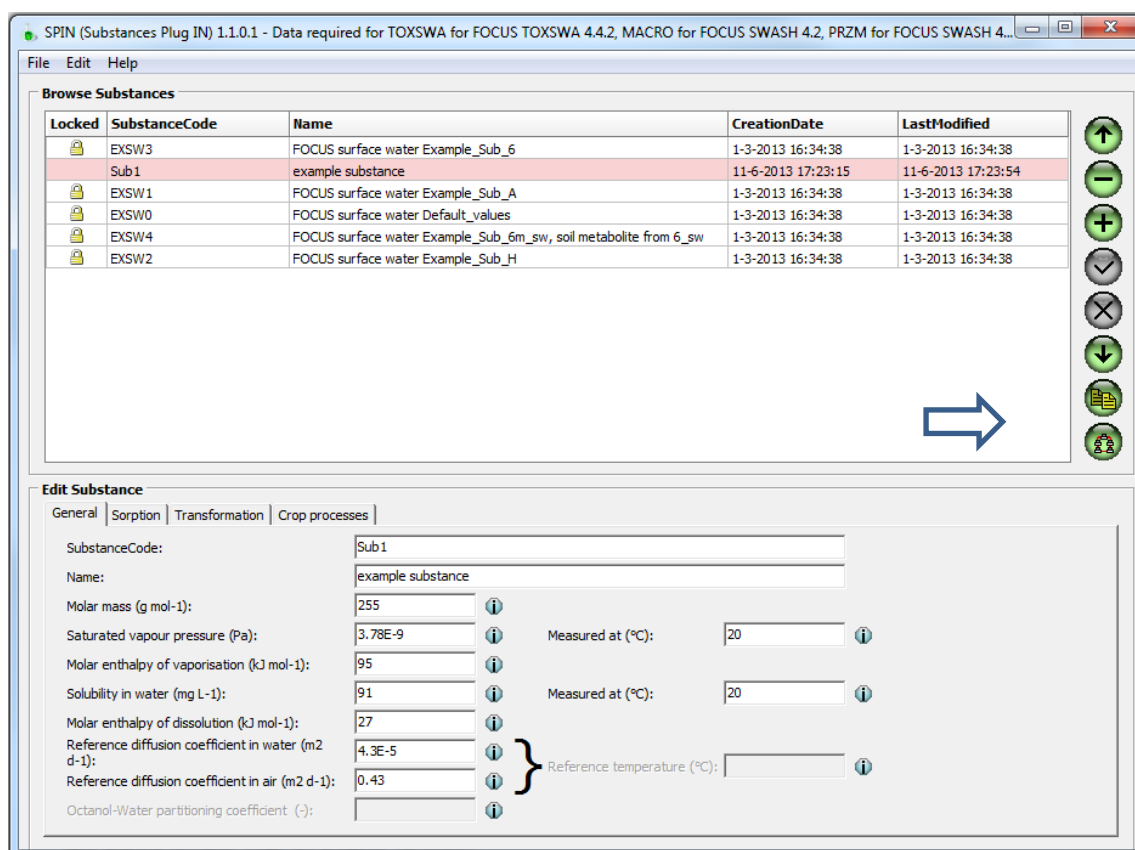


Figure 13: The metabolite button provides access to the metabolite form that enables the linking of metabolites to parent substances.

The metabolite window, as shown in Figure 14, is divided in four tabs: Soil, Surface water, Sediment and Recirculation water. These tabs represent the different compartments where the metabolite(s) can be formed. Recirculation water refers to Greenhouses and is not relevant to FOCUS_SWASH and FOCUS_TOXSWA. Each table is divided in two parts:

- the **Browse metabolites** part. Here, all metabolites associated to a parent substance are shown. The buttons on the right hand-side have the same functionality as described in Section 2.2.3. The buttons appear in a grey colour when their functionality is disabled, otherwise they appear in green.
- the **Edit metabolites** part. A metabolite from a drop-down menu can be selected and the fraction transformed can be entered.

The user has to select the appropriate compartment tab, and then the metabolite can be added using the  button on the right hand side. Now the user can select the metabolite from the drop-down menu and the fraction transformed in the compartment can be entered.

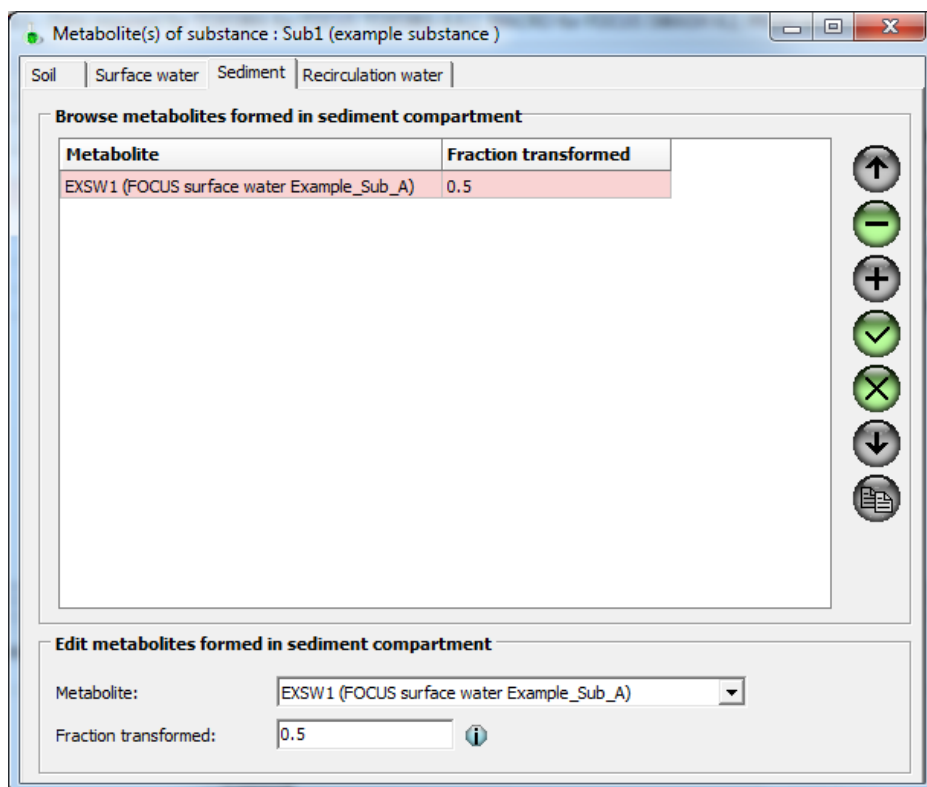


Figure 14: The metabolite(s) window. This window enables the creation and editing of metabolites in the compartments Soil, Surface Water, Sediment and Recirculation Water (greenhouses).

For complex metabolite schemes it is advised to make a matrix scheme, for each compartment, like the example in Table 1, to keep an overview.

Table 1: Example of a matrix which represents the reactions between the compounds included in the reaction scheme of a pesticide. 0 = no reaction. χ = molar fraction of a compound transformed into a specific product (after Leistra et al., 2001).

	Parent	Product 1	Product 2	Product 3	Product 4	Product 5
Parent	0	$\chi_{p,1}$	$\chi_{p,2}$	0	0	0
Product 1	0	0	0	$\chi_{1,3}$	$\chi_{1,4}$	0
Product 2	0	0	0	0	0	0
Product 3	0	0	0	0	0	$\chi_{3,5}$
Product 4	0	0	0	0	0	$\chi_{4,5}$
Product 5	0	0	0	0	0	0

5 Export or import substance properties

SPIN facilitates export and import of substances to and from text files. These options are explained below. Note that it is not possible to export or import metabolite schemes.

5.1 Data export

In the Menu Bar, the user can select the File / Export option. Subsequently, the user may choose between the export of substance properties or the export of substance meta-data (Figure 15). The latter consists of a list of all properties in SPIN. For each property the substance ID, substance name, unit, caption, description, minimum value, maximum value, default value (always empty) and data type (e.g. float, integer, boolean) is given.

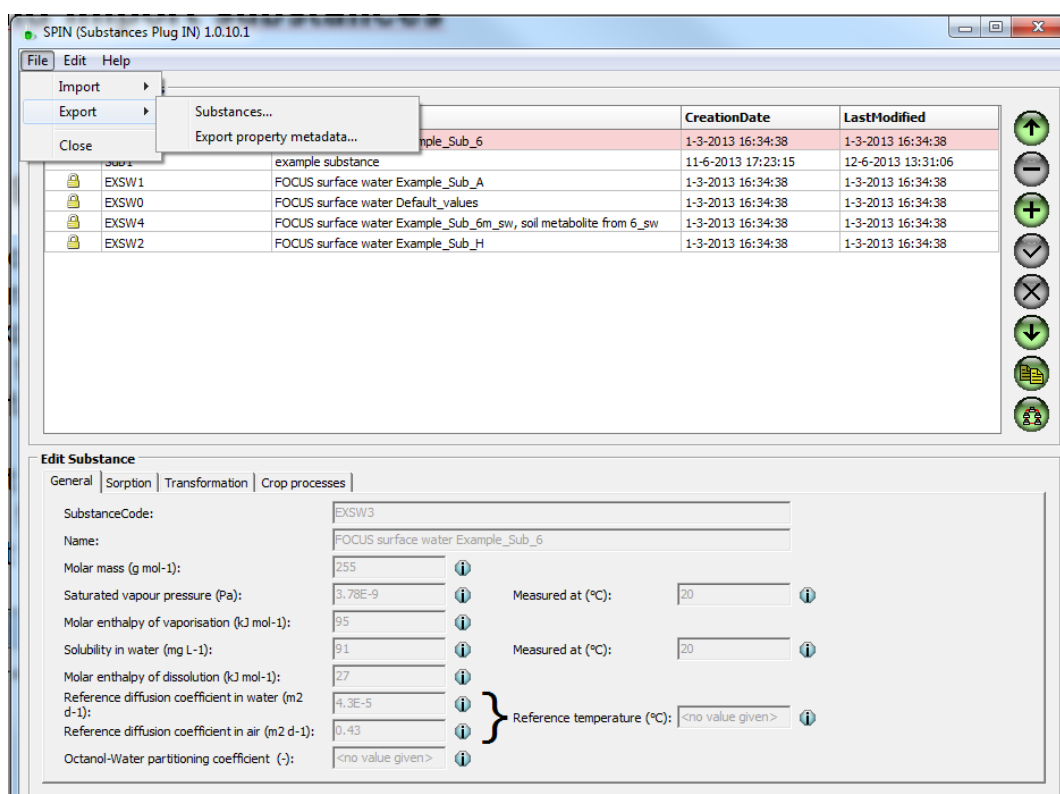


Figure 15: Export selection option to export substance properties and metadata.

For both the export of substance properties and the export of metadata, the user may choose the separator between fields and the decimal separator (Figure 16). After selection of the separators a window opens to select the export directory and file name.

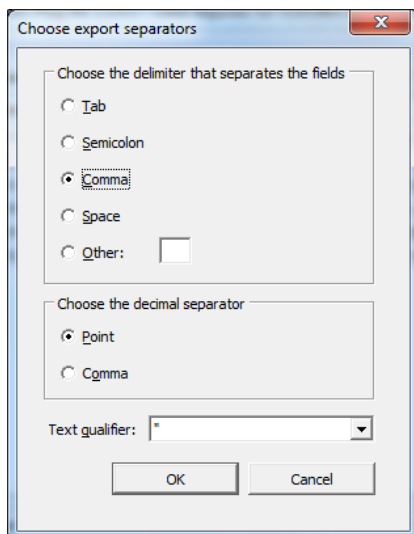


Figure 16: The Choose export separator form allows to select the separators.

5.2 Data import

In the menu, one can select the File / Import / Substances option. A window opens to select the import file. Then a window pops up that enables the delimiter selection and a preview of the interpreted data. SPIN checks the validity of the imported data for each field. In case SPIN detects an inconsistency, an error message pops up (Figure 17). The affected cells are marked in red.

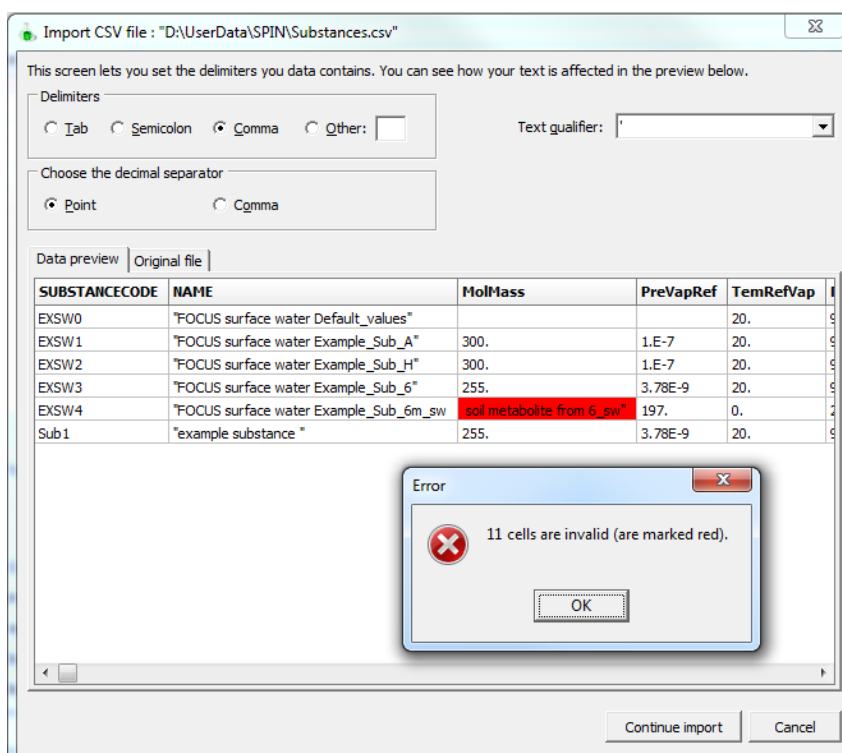


Figure 17: The import substances window enables the selection of delimiters and the preview of data. An error message pops up in case of inconsistencies in the imported data.

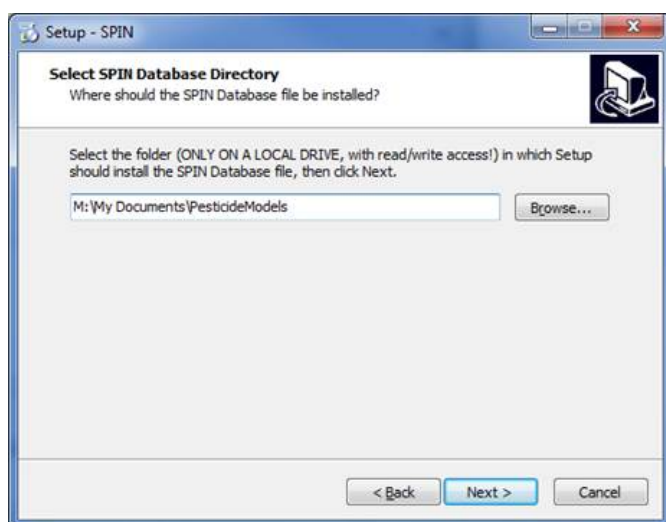
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Appendix 1 Installation procedure for multiple users

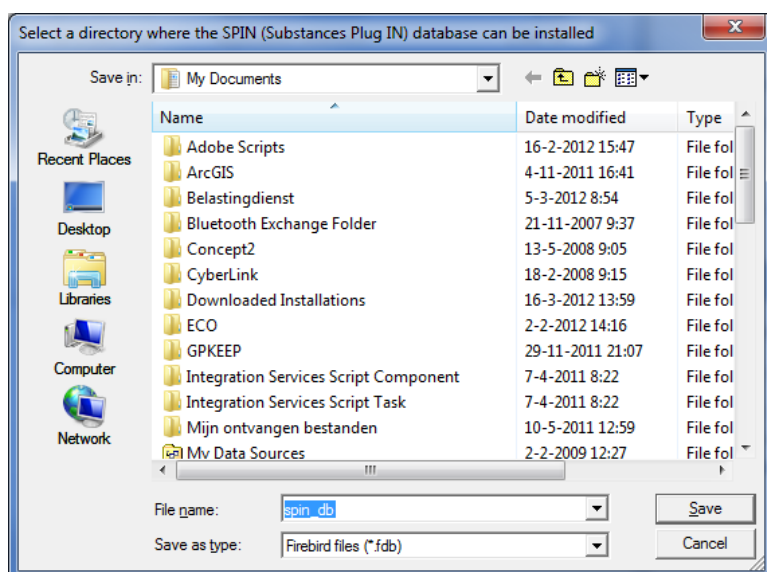
If multiple users on one PC or Laptop want to use SPIN it is only necessary to install SPIN once.

The first user installs SPIN and should have administrator privileges. During the installation process this user has the option to select the directory of the SPIN database.



- In case each user should have its own SPIN database select a user specific directory where only the user itself has access to.
- In case each user should use the same SPIN database select a 'common' directory where every user had read/write access.

The second user doesn't need to install SPIN again. However the first time SPIN is started the user has to indicated where the SPIN database is located.



- In case the user wants to use its own database select a user specific directory and a new empty SPIN database will be installed on that directory.
- In case the user wants to use the same database as the first user select the directory where the first user installed the SPIN database.

The selected location is saved in the registry of the (second) user. This means this window only appears the first time SPIN is started.

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