



## FRENCH REFINEMENT OF GROUNDWATER SCENARIOS (VERSION 3.3.3.3)

### **FROGS Interface User Manual**

Beigel, C.<sup>1</sup>, Berardozi, M.<sup>2</sup>, Cecchi, M.<sup>3</sup>, Domange, N.<sup>4</sup>, Garcia, L.<sup>5</sup>, Guyot, C.<sup>6</sup>,  
Hammel, K.<sup>7</sup>, Schubert, S.<sup>8</sup>, Kahl, G.<sup>10</sup>, Knowles, S.<sup>9</sup>, Loiseau, L.<sup>2</sup>, Obeidy, C.<sup>3</sup>,  
Reiher, W.<sup>10</sup>, Shbaita, H.<sup>5</sup>

9 January 2014

<sup>1</sup>BASF, Singapore; <sup>2</sup>Syngenta, Switzerland; <sup>3</sup>Syngenta Agro, France; <sup>4</sup>ONEMA, France;  
<sup>5</sup>BASF, Germany; <sup>6</sup>Bayer CropScience, France; <sup>7</sup>Bayer CropScience, Germany; <sup>8</sup>Dow  
AgroSciences, Germany; <sup>9</sup>Dow AgroSciences, UK; <sup>10</sup>Dr. Knoell Consult, Germany

# **FROGS Interface User Manual**

## **TABLE OF CONTENTS**

1	Introduction.....	3
2	Software Requirements .....	3
3	FROGS distribution content and installation .....	4
4	Running the program .....	5
4.1	Application settings .....	7
4.2	Add/Edit substance .....	9
4.2.1	Substance management .....	10
4.2.2	Editing substance properties .....	12
4.2.3	Adding/Editing transformation schemes .....	13
4.3	Add/Edit application scheme .....	14
4.3.1	Add/Editing application schemes.....	16
4.3.2	Add/Editing applications .....	17
5	Anatomy of a generated simulation run .....	19
5.1	Catalogue.txt.....	21
5.2	run.bat.....	22
6	Evaluation of a completed run .....	23

# 1 Introduction

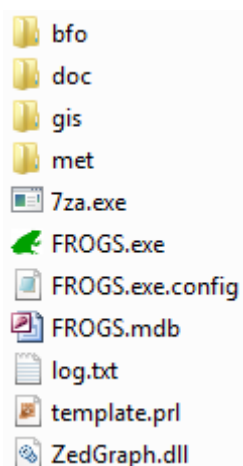
This document refers to version 3.3.3.3 of the FROGS interface. The graphical user interface (GUI) presented in present document enables the user to generate and evaluate FOCUS-PEARL 4.4.4 runs based on the FROGS scenarios. The GUI is linked with a relational database where parameters on soils, crops, substances, and application scenarios are stored. Substance parameters and application scenarios can be edited through the GUI. Additionally, information is stored in ASCII-files in subdirectories of the FROGS distribution folder (weather files, pre-run hydrology). The PEARL model is used for running FROGS. However, FOCUS scenario data, whilst contained within the FOCUS-PEARL 4.4.4 database, are not used as part of FROGS.

## 2 Software Requirements

- The FROGS GUI was tested successfully on different blends of **Microsoft Windows** (NT/2000, Server 2003, XP, Vista, 7, Windows 7). It will not run under Linux or MacOS.
- The FROGS GUI requires **Microsoft .NET Framework 2.0** (or higher). The .NET framework can be downloaded freely from <http://www.microsoft.com>
- Free hard disk space: The entire FROGS **distribution takes up 9.3 GB** of hard disk space. A completed run with all result files can take up > 8.4 GB without bfo files (parent + one metabolite).
- **FOCUS-PEARL 4.4.4** must be installed. FOCUS-PEARL 4.4.4 can be freely downloaded from <http://focus.jrc.ec.europa.eu/gw/index.html>


### 3 FROGS distribution content and installation

Figure 1 shows the files and folders found in the FROGS distribution, while their definitions are presented in Table 1.



**Figure 1 Contents of the distribution directory**

**Table 1 Files/Folders of the FROGS distribution**

File/Folder	Definition
doc	Documentation files
gis	Agronomic Units shape file
met	Weather files for Pearl (*.met)
bfo	Pre-run hydrology files (*.bfo) for each scenario compressed into 7z-archives
7za.exe	Compression program to extract pre-run hydrology files
 FROGS.exe	<b>FROGS GUI main executable</b>
FROGS.exe.config	Configuration file for FROGS.exe in XML-format. Editable in standard text editor or from settings menu within FROGS.exe shell
FROGS.mdb	Microsoft Access database containing scenario definitions
log.txt	Error logging file for FROGS.exe
template.prl	PEARL input template file
ZedGraph.dll	Software library for charting functionality

To install FROGS, create a new folder on a hard drive, for example C:\FROGS, and extract/copy the content of the distribution directory in it.

## 4 Running the program

The procedure for generating and evaluating FROGS scenarios is shown in the following graph (Figure 2).

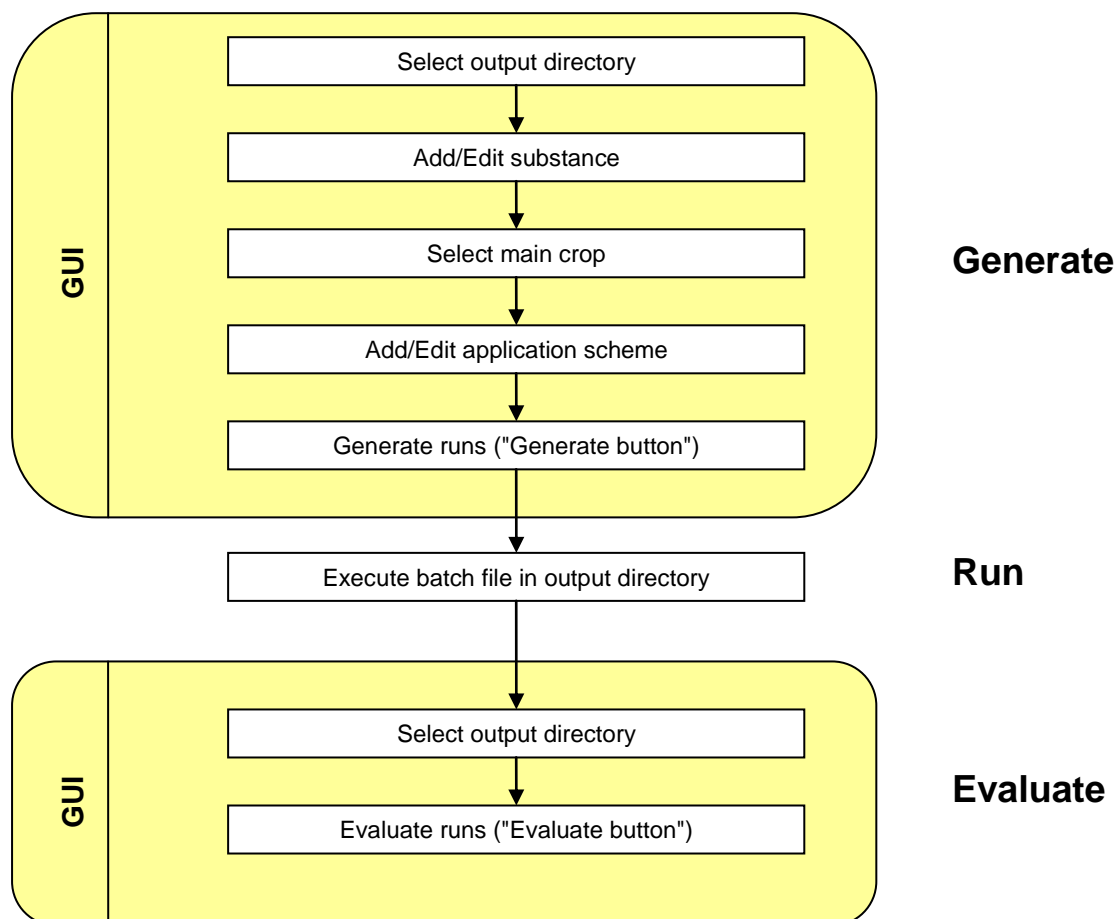



Figure 2 Steps involved in running FROGS

The main executable that starts up the main form of FROGS GUI is  FROGS.exe (Figure 3).

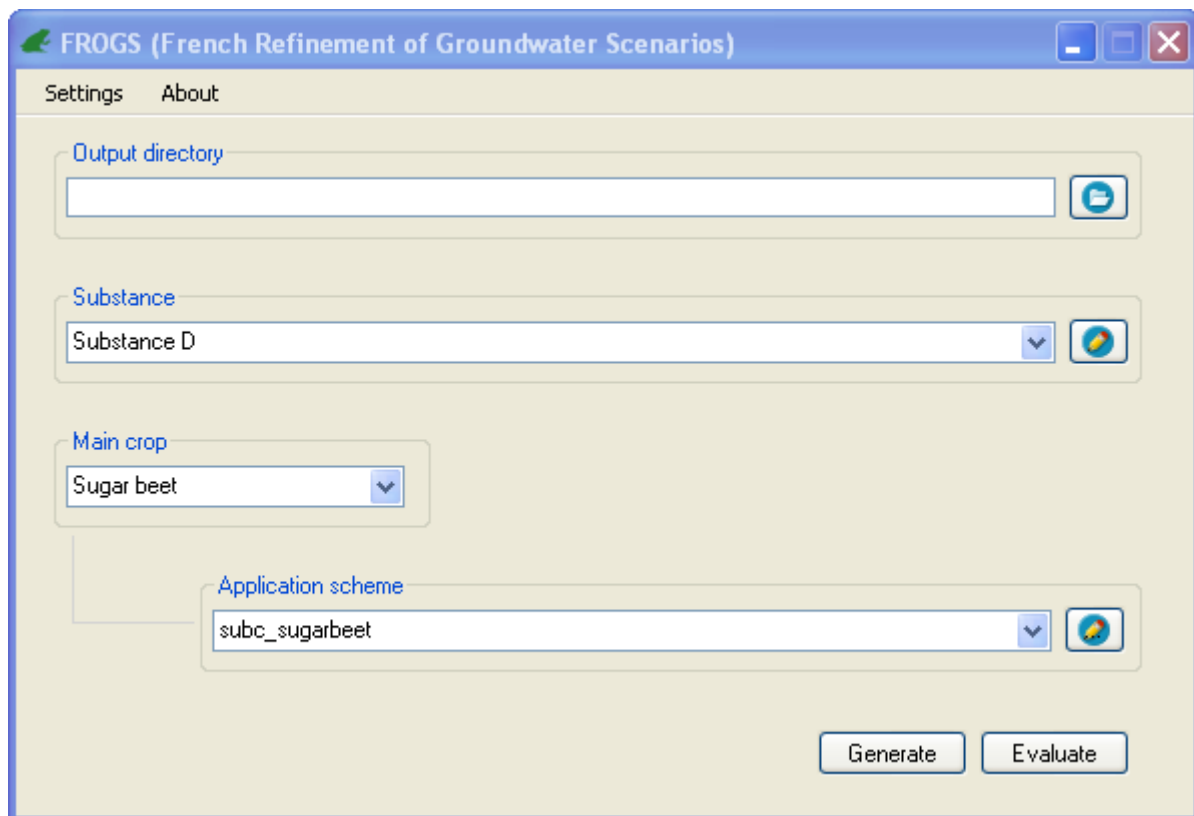


Figure 3 FROGS main form

## 4.1 Application settings

Through menu item *Settings* on the main form basic application setting can be configured (Figure 4). Set the path to the `pearlmodel.exe` at your local system or copy in the `pearlmodel.exe` and `SWAP3234.exe` from your PEARL 4.4.4 installation path (both files can be found in the bin-folder of your local PEARL installation).

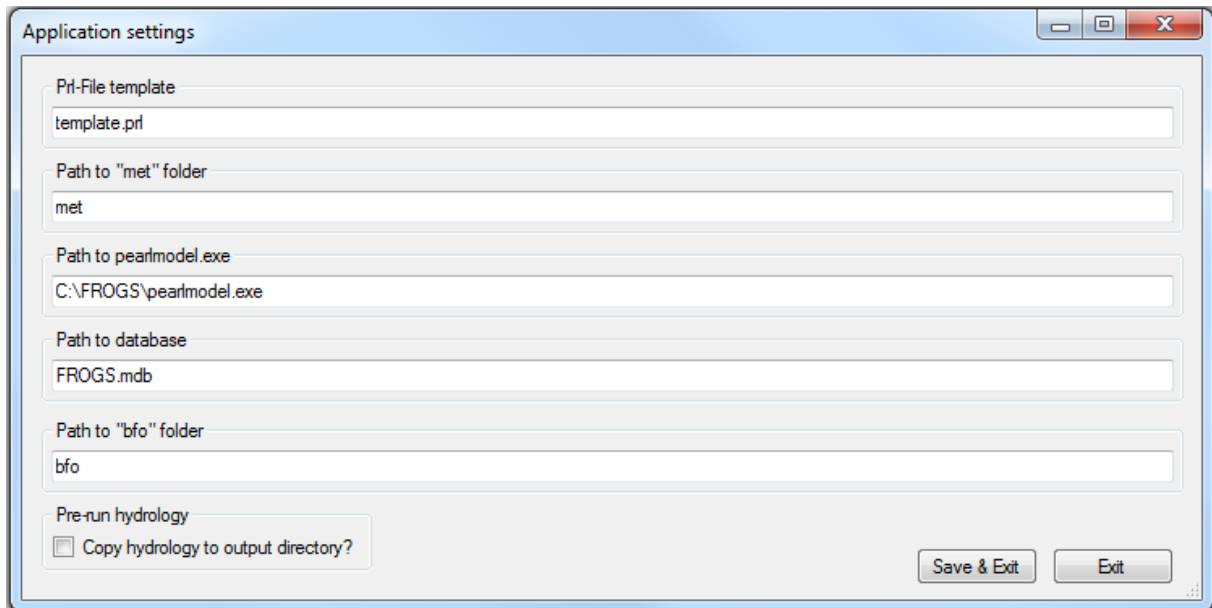


Figure 4 Application settings form (*MainForm* → *Settings*)

### Prl-File template

Pearl input files (\*.prl) are generated from a template file where the parameters making up a FROGS run are inserted. Below an extract from the template file is presented (Figure 5). Sections that are replaced by FROGS GUI are encompassed by # (example: #MeteoStation# is replaced by the name of the weather file).

```
*-----
* Section 3: Weather and irrigation section
*-----

#MeteoStation#      MeteoStation
Input               OptEvp
1                   FacPrc (-)
0                   DifTem (C)
1                   FacEvp (-)
2.35               TemLboSta      (C)
Daily               OptMetInp
No                  OptRainfallEvents
No                  OptSnow
Laminar             OptTraRes

#Irrigation#
```

Figure 5 Extract from file `template.prl`

#### Path to "met" folder

A relative (e.g. relative to *FROGS.exe*) or absolute path to the folder where the weather files (\*.met) are located. Default location is subdirectory *met* in the FROGS distribution.

#### Path to pearlmodel.exe

A relative (e.g. relative to *FROGS.exe*) or absolute path to the main executable of FOCUS-PEARL 4.4.4.

#### Path to database

A relative (e.g. relative to *FROGS.exe*) or absolute path to the database in which the FROGS scenarios are defined.

#### Path to "bfo" folder

A relative (e.g. relative to *FROGS.exe*) or absolute path to the folder where the pre-run hydrology is stored. Because of their size, bfo-files are compressed in 7z-archives. FROGS GUI takes care of extraction and renaming so that FOCUS-PEARL can read it.

Contrary to earlier versions FROGS 3.3.3.3 is parameterized in such a way that it requires the pre-run hydrology files. Otherwise the calculation of the pre-run hydrology would require too much time. Users wishing to calculate the pre-run hydrology on their own for any reason (not recommended for standard FROGS scenarios but could be relevant for any further higher tier options that affect the soil hydrology), are advised to change the entry for variable "OptHyd" in the section 1 of template.prl file from "Offline" into "Automatic".

#### Pre-run hydrology

If box is checked pre-run hydrology files are copied into the project directory. This may be useful when runs should be transferred to other computers.



## 4.2 Add/Edit substance

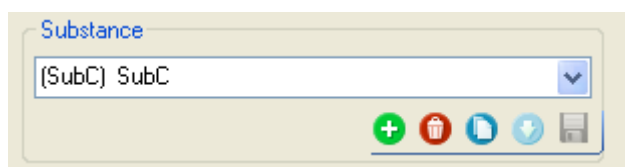
The substance form (Figure 6) can be accessed by clicking on the Substance-🌐 in the FROGS main form.

[illegible]

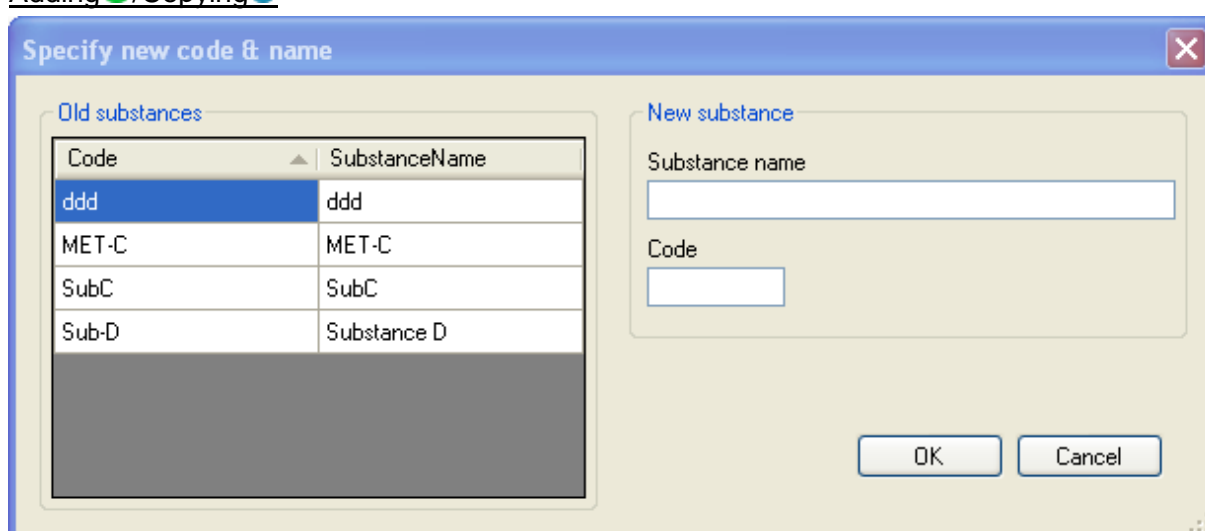
**Figure 6 Substance Form (MainForm → Substance-📌)**

## 4.2.1 Substance management

Substances can be added<sup>+</sup>, deleted<sup>✖</sup>, copied<sup>📄</sup>, and imported<sup>📥</sup> from an existing prl-input file.



### Adding<sup>+</sup>/Copying<sup>📄</sup>



**Figure 7 Adding/Copying new substance**

When adding/copying a new substance the user has to provide a substance name and a unique code. To ensure that the code is not already assigned the left-hand control lists all the substances that are already contained in the database.

### Deleting<sup>✖</sup>

Delete the currently selected substance in the database.

### Importing<sup>📥</sup>

FROGS GUI provides the possibility to import substances from an existing prl-input file generated from previous FOCUS Pearl 3.3.3 or 4.4.4 runs.

On the import form (Figure 8) a prl-file can be specified. If the specified file is in a correct format the form automatically reads in all substance parameters for all substances found in the file. Subsequently, the form lists all substances of the file in the left-hand list box.

To review the parameters before finally importing them into the database, a substance can be selected in the left-hand list box. Parameters are then shown in the *Details* text box.

Button *Accept* writes all substances into the database.

#### Limitations of the import form:

- Transformation schemes (e.g. formation fractions) are presently not imported
- Substances can only be imported when the substance code is not already included in the database. In that case the original prl-file could be opened in a standard text editor (for example notepad) and the occurrences of the substance code could be replaced with a unique one.
- The substance name of the imported substance is set to the substance code.

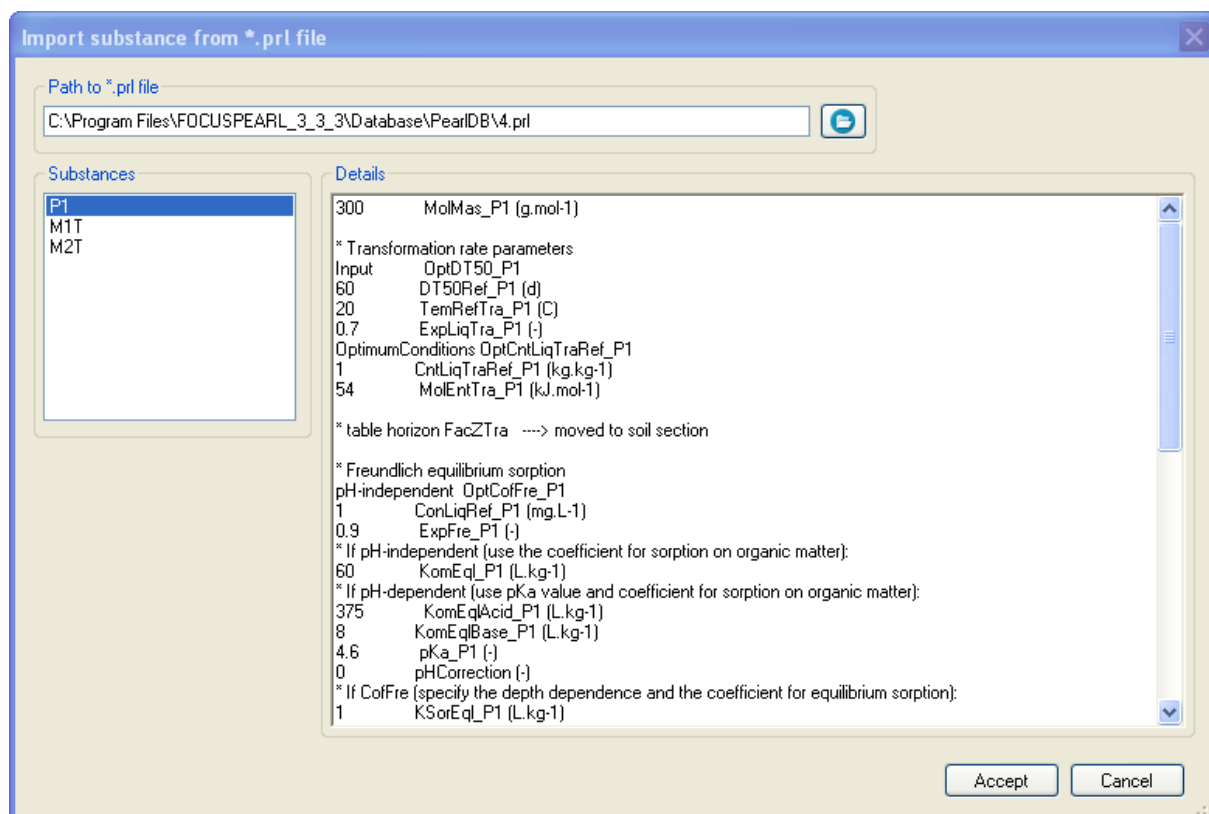

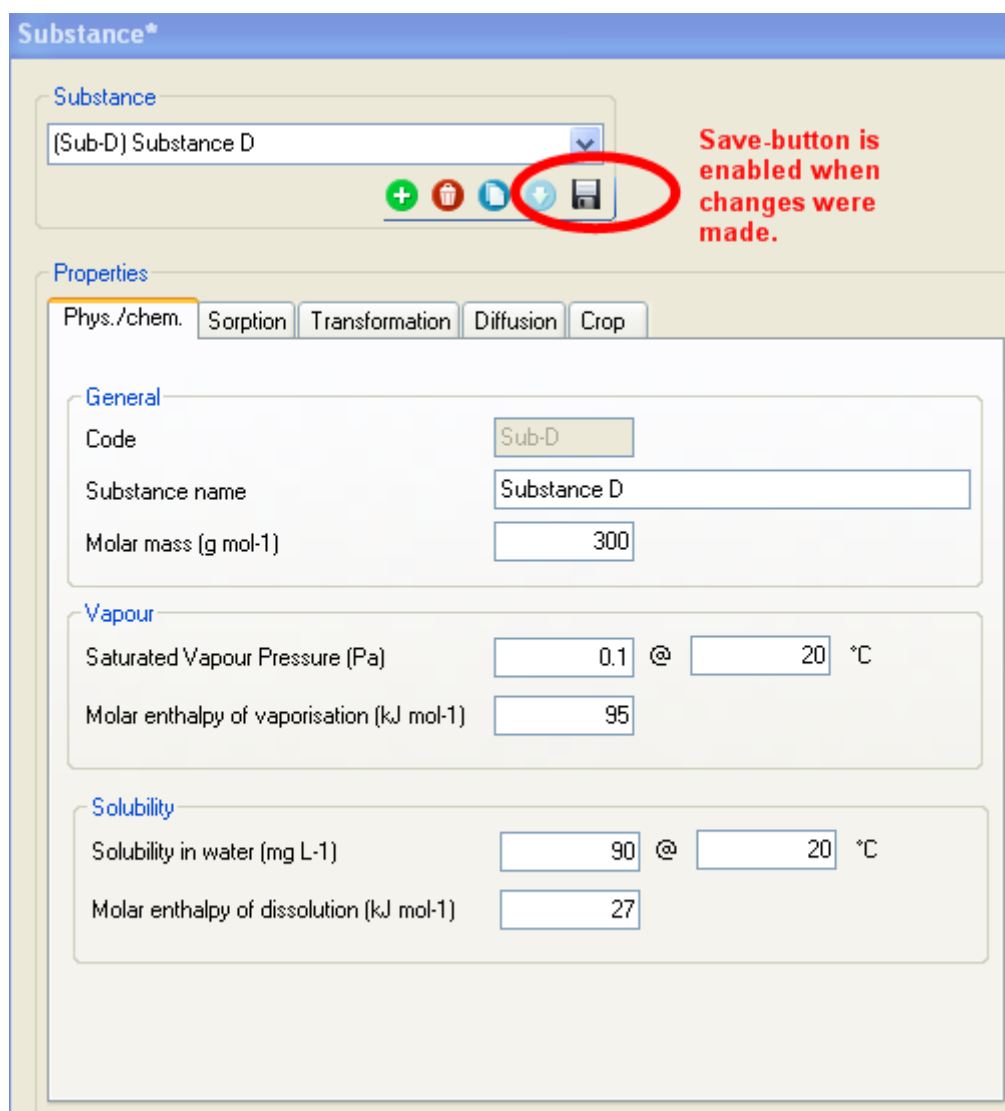


Figure 8 Importing substance from existing prl-file.

## 4.2.2 Editing substance properties

The four substance property categories phys./chem., sorption, transformation, diffusion, and crop can be edited in the respective tabs (Figure 9). If changes were made to the properties the Save-button  is enabled. In order to write the changes permanently to the database this button has to be pushed.



The screenshot shows the 'Substance\*' application window. At the top, there is a 'Substance' section with a dropdown menu showing '[Sub-D] Substance D'. Below this are five icons: a green plus sign, a red trash can, a blue document, a blue download arrow, and a black floppy disk (Save icon). The Save icon is circled in red. To the right of this circle, red text reads: 'Save-button is enabled when changes were made.' Below the icons is a 'Properties' section with five tabs: 'Phys./chem.', 'Sorption', 'Transformation', 'Diffusion', and 'Crop'. The 'Phys./chem.' tab is selected. It contains three sub-sections: 'General' with fields for 'Code' (Sub-D), 'Substance name' (Substance D), and 'Molar mass (g mol<sup>-1</sup>)' (300); 'Vapour' with fields for 'Saturated Vapour Pressure (Pa)' (0.1), '@' (20 °C), and 'Molar enthalpy of vaporisation (kJ mol<sup>-1</sup>)' (95); and 'Solubility' with fields for 'Solubility in water (mg L<sup>-1</sup>)' (90), '@' (20 °C), and 'Molar enthalpy of dissolution (kJ mol<sup>-1</sup>)' (27).

Figure 9 Saving changes to substance properties.

### 4.2.3 Adding/Editing transformation schemes

Transformation schemes, e.g. the formation of metabolites, can be added<sup>+</sup>, edited<sup>🎨</sup>, and deleted<sup>🗑️</sup> on the right-hand side of the Substance-form (Figure 6, Figure 10). Unlike other substance properties (phys/chem., sorption, transformation, diffusion, and crop) changes to transformation schemes have not to be confirmed by the Save-button<sup>💾</sup>.

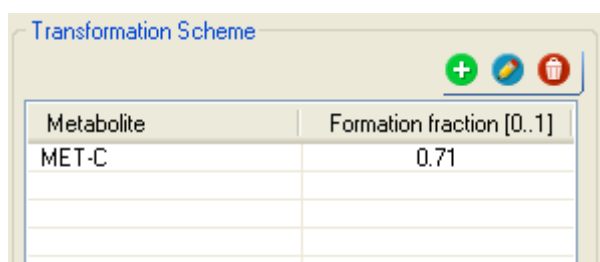


Figure 10 Formation of metabolites

#### Adding<sup>+</sup>

The form *Add metabolite* (Figure 11) allows to select any other substance contained in the database as metabolite.

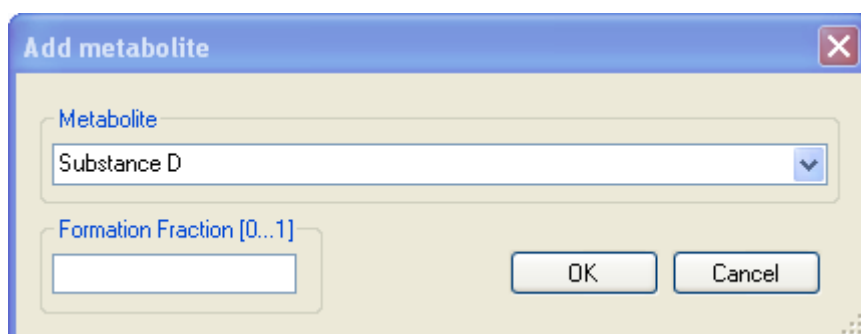
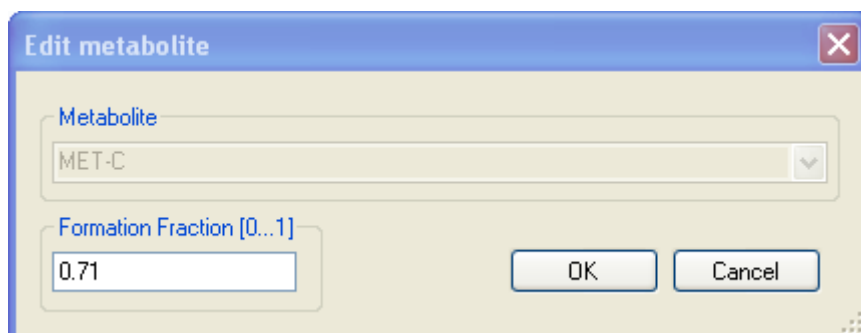


Figure 11 Adding a metabolite to a substance

#### Editing<sup>🎨</sup> (can be also called by double-click on list entry)

Allows to edit the formation fraction of an existing metabolite.



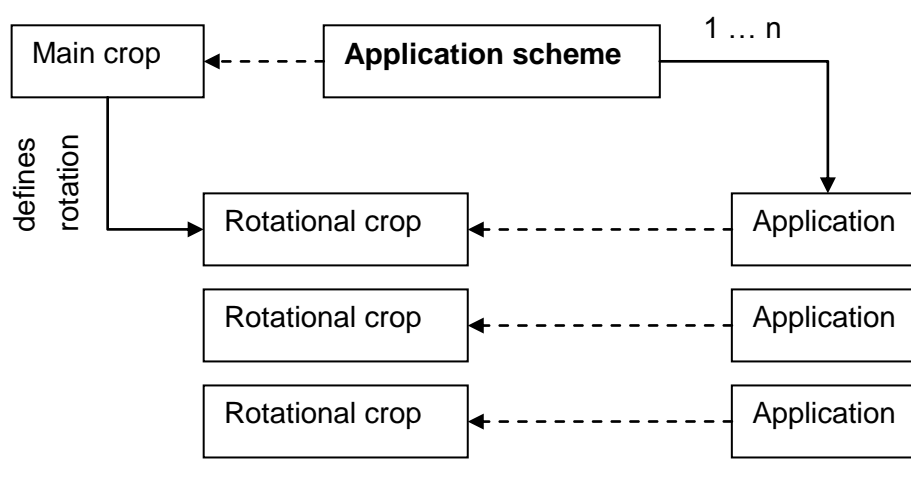
#### Deleting<sup>🗑️</sup>

Deletes the currently selected transformation in the database.

### 4.3 Add/Edit application scheme

Applications of substance are organized in application schemes (Figure 12). Each application scheme is linked to a main crop as defined in FROGS. This is necessary in order to obtain all crops that occur in rotation with the main crop. Each individual application is linked to one of those rotational crops.

Rotational schemes representative of the different French geo-climatic regions are implemented automatically in FROGS. Once a main crop is selected, the crops with which it is typically rotated are set automatically. The user has to specify applications to the main crop in the rotation pattern and it is initially assumed that no applications are made to the other crops. In case applications are also made to one or several of the other crops appearing in the rotations, the user has to add separate applications for each of these crops. It is recommended to first add in the application form the application(s) to the main crop, then add the application(s) to rotational crops if relevant (to add applications, see 4.3.2).



**Figure 12 Relationship between application scheme, applications, and crops**

For setting up application schemes the Application-Form is intended (Figure 13).

Applications

Application scheme

subc\_sugarbeet

+

✖

📄

Main crop:

Sugar beet

Applications

+

✏

✖

Crop	Soil load (kg/ha)	Type	Detail 1	Detail 2	Detail 3
Sugar beet	0.35	relative	Emergence	0 days	

...

Definitions for Detail 1, 2, and 3:

Absolute app.: 1) Date of app.; 2) First or second year app.; 3) -

Relative app.: 1) Crop event; 2) Relative days; 3) -

BBCH app.: 1) BBCH code; 2) Relative days 3) Consider Fall/Spring only

Figure 13 Add/Edit application schemes and applications.

15

### 4.3.1 Add/Editing application schemes

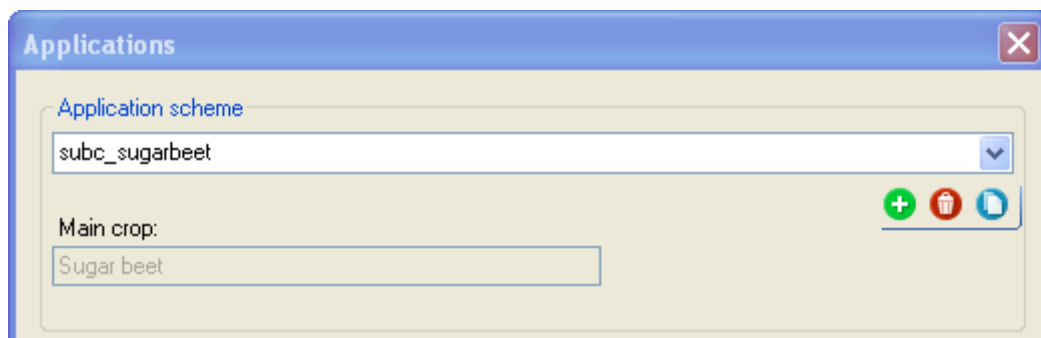


Figure 14 Application scheme management

#### Adding

A new application scheme name and the main crop have to be provided (Figure 15).

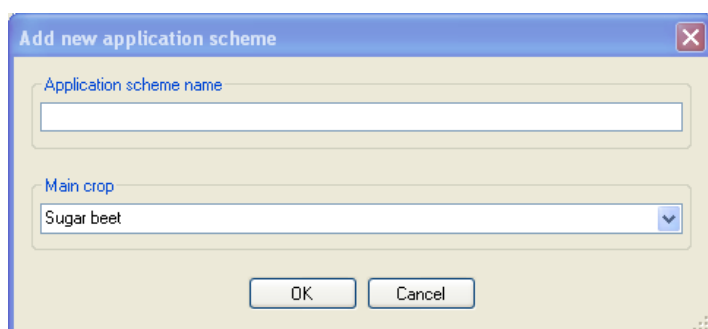


Figure 15 Add new application scheme

#### Deleting

Delete the current application scheme.

#### Copying

For creating a copy of an existing application scheme, first open the application scheme to be copied, then click on the copy button, and simply provide a new name for the new application scheme.

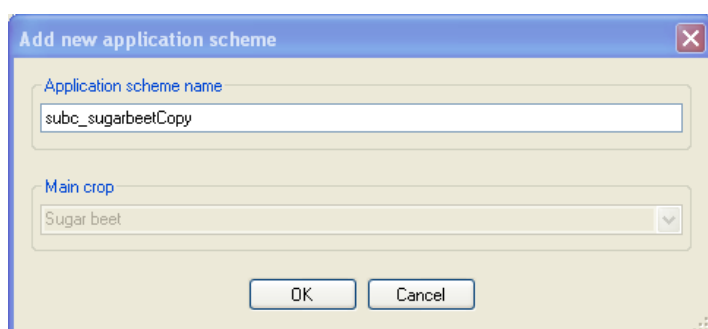
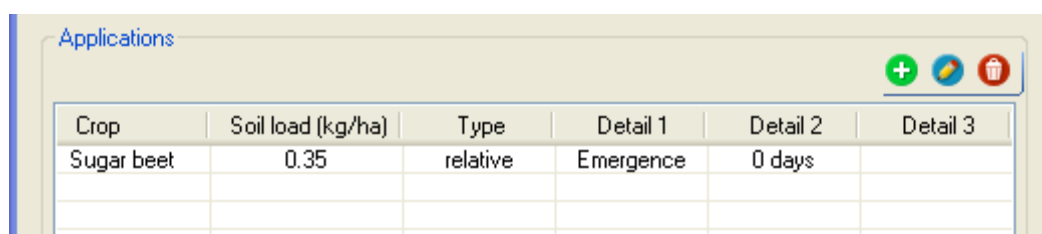


Figure 16 Create copy of an existing application scheme.



### 4.3.2 Add/Editing applications

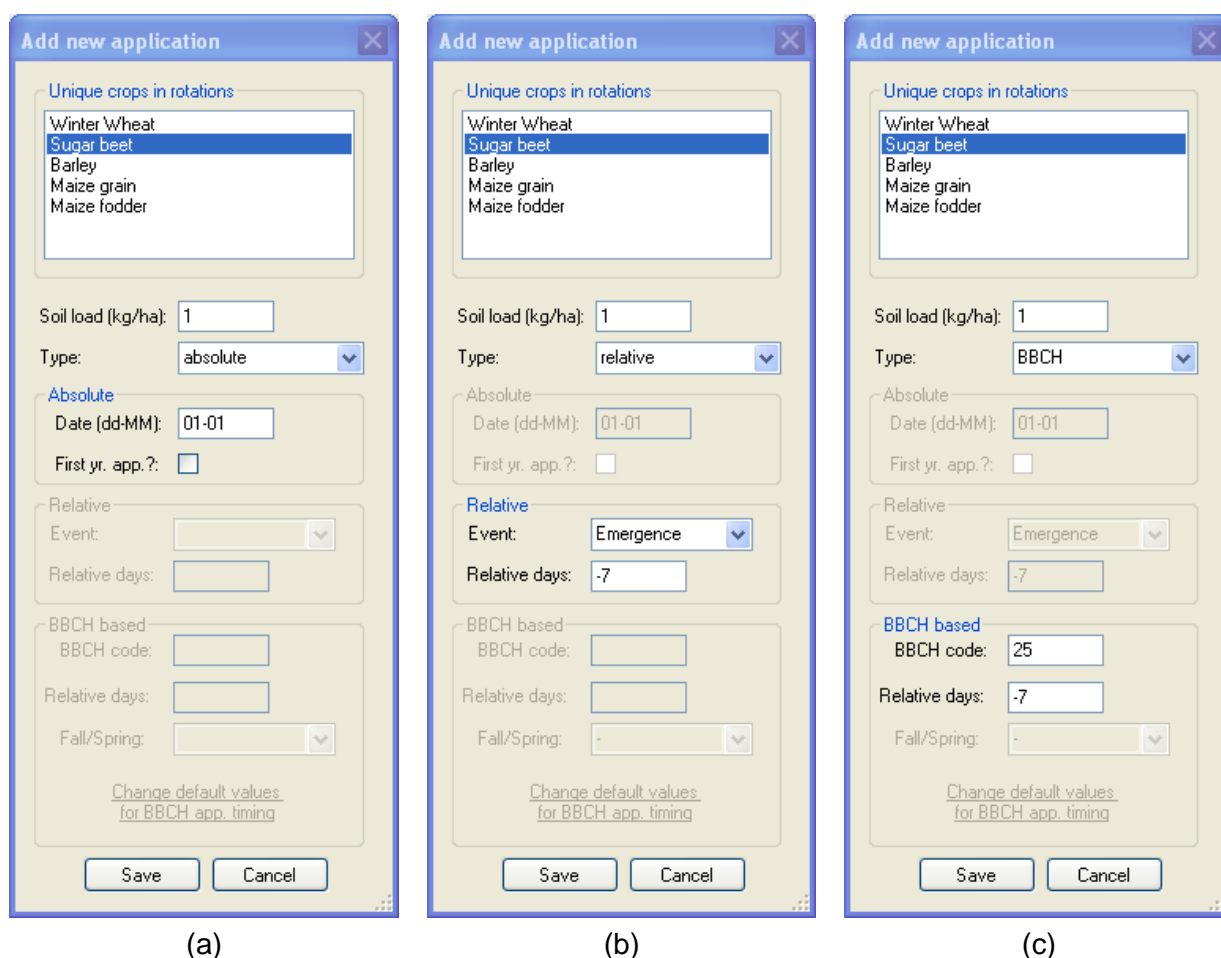


Crop	Soil load (kg/ha)	Type	Detail 1	Detail 2	Detail 3
Sugar beet	0.35	relative	Emergence	0 days	

Figure 17 Application management

#### Adding /Editing

For adding/editing an application, select the relevant crop (main crop or rotational crop), select application type between absolute, relative, BBCH, and the following form shows up, depending on the selected application type (Figure 18).



(a)

(b)

(c)

Figure 18 Add/Edit applications: (a) absolute, (b) relative, and (c) BBCH-based application timing

Unique crops in rotation: Crops that occur in rotation with the selected main crop. An application is always linked to a rotational crop.

Soil load (kg/ha): Substance reaching soil, e.g. soil load application rate - interception

Type: Application timing type: absolute, relative, or BBCH. For details see below.

There are three different application timing types implemented in FROGS GUI:

absolute: Day and month (format "day-month") of the application date have to be specified. For each year when the crop, onto which the application is to be applied, an application written to the prl-file.

A special case arises with biennial crops like winter wheat. In order to specify whether the application occurs in the first or second year the flag "*First yr. app?*" has to be set. If set it indicates that the application occurs in the first year.

relative: Applications are scheduled relative to a crop date like emergence, e.g. the combination *Event = Emergence* and *Relative days = -7* sets the application one week before emergence date.

BBCH: Applications are scheduled relative to when a crop reaches the specified growth stage (BBCH based), e.g. the combination *BBCH = 25* and *Relative days = -7* sets the application to one week before a crop reaches growth stage 25 in an Agronomic Unit.

#### Limitations of BBCH based application timing:

- The option *Fall/Spring* is not implemented, yet.
- Growth stages are simulated with the help of a phenology model implemented in FROGS GUI. However, emergence dates, the starting points for the growth stage simulations, are the same for all years.
- When generating the runs and encountering a BBCH based application timing the aforementioned phenology model is run internally. This may increase the duration for the generation of the runs for a few minutes.

Deleting 

Delete the selected application.

## 5 Anatomy of a generated simulation run

Button *Generate* on the main form produces all the input files necessary to run a FROGS simulation based on the selections made for substance, main crop, and application scheme in the specified output directory.

Name	Size	Type
1.prl	31 KB	PRL File
1.SWE	0 KB	SWE File
2.prl	32 KB	PRL File
2.SWE	0 KB	SWE File
3.prl	32 KB	PRL File
3.SWE	0 KB	SWE File
4.irr	1 KB	IRR File
4.prl	31 KB	PRL File
4.SWE	0 KB	SWE File
5.prl	31 KB	PRL File
5.SWE	0 KB	SWE File
...		
7.SWE	0 KB	SWE File
7za.exe	524 KB	Application
...		
53050.met	580 KB	MET File
...		
AUID 31 SID 8 CID 2.7z	3,274 KB	WinRAR-Archiv
AUID 31 SID 9 CID 2.7z	3,295 KB	WinRAR-Archiv
AUID 31 SID 12 CID 2.7z	3,166 KB	WinRAR-Archiv
AUID 31 SID 13 CID 2.7z	3,581 KB	WinRAR-Archiv
AUID 31 SID 19 CID 2.7z	3,299 KB	WinRAR-Archiv
catalogue.txt	4 KB	Text Document
run.bat	33 KB	MS-DOS Batch File

Figure 19 Anatomy of a FROGS simulation run

**Table 2 Definition of files generated in the output directory, e.g. FROGS simulation run**

File(s)	Definition
*.prl	Main Pearl input files
*.swe	Empty file that Pearl requires to run the pre-run hydrology
7za.exe	<p><u>This file is only present when "Copy pre-run hydrology" property is checked on the settings form.</u></p> <p>Executable to decompress pre-run hydrology files (*.pfo) that are contained in 7z-archives (*.7z)</p>
*.met	Weather file
*.7z	<p><u>These files are only present when "Copy pre-run hydrology" property is checked on the settings form.</u></p> <p>Compression archive that contains pre-run hydrology for each scenario. Naming convention makes use of primary keys from database for agronomic units (AUID), soils (SID), and main crop (CID)</p>
catalogue.txt	Summary of scenario definitions (details follow below)
run.bat	Batch file to start the simulation

One scenario, i.e. "agronomic unit-soil-main crop" combination is uniquely defined by

- one \*.prl file
- one \*.met file
- one \*.swe file
- one \*.7z file

## 5.1 Catalogue.txt

Catalogue.txt summarizes all the scenarios. The file is intended for informative purposes but is also mandatory for evaluation after the runs are completed.

```

1 2 CID_MAIN
2 4 5 6 SUBID
3 17 APPSCHEMEID
4 RunID AUID SID MET
5 1 1 1 43044
6 2 2 1 52041
7 3 4 1 57048
8 4 5 1 51055
9 5 6 1 55044
10 6 8 1 43043

```

**Figure 20 Extract from catalogue.txt**

**Table 3 Definition of lines found in catalogue.txt**

Line#	
1	Primary key of the main crop (tblCrops in database)
2	Primary keys of substances (tblSubstance in database); first is parent
3	Primary key of application scheme (tblApplicationScheme in database)
4	Header
5 ... n	Run-IDs and primary keys of agronomic units (AUID), soils (SID), as well as name of weather file (*.met) Example: Line 5 defines the run that comprises files "1.prl", "1.swe", "AUID 1 SID 1 CID 2.7z"

## 5.2 run.bat

Batch file to start the simulation. Each scenario requires several lines in the batch file. Depending on the option "Copy pre-run hydrology" in the main settings (see section 4.1 Application settings) a batch file looks differently:

### Option "Copy pre-run hydrology" enabled

```
7za.exe e "AUID 3 SID 2 CID 1.7z"
RENAME "AUID 3 SID 2 CID 1.bfo" 1.bfo
"C:\FROGS\pearlmodel.exe" 1
DEL /Q 1.bfo
...
```

Figure 21 Extract from run.bat with option "Copy pre-run hydrology" enabled

Table 4 Definition of lines found in run.bat

Line#	Definition
1	Extract pre-run hydrology file from archive, which resides in the same directory
2	Rename extracted pre-run hydrology file to the name of the respective *.prl file
3	Execute simulation
4	After simulation has completed delete pre-run hydrology file

### Option "Copy pre-run hydrology" disabled

```
"C:\FROGS\7za.exe" e "C:\FROGS\bfo\AUID 3 SID 2 CID 1.7z"
RENAME "AUID 3 SID 2 CID 1.bfo" 1.bfo
"C:\FROGS\pearlmodel.exe" 1
DEL /Q 1.bfo
...
```

Figure 22 Extract from run.bat with option "Copy pre-run hydrology" enabled

Table 5 Definition of lines found in run.bat

Line#	Definition
1	Extract pre-run hydrology file from archive located at specified path
2	Rename extracted pre-run hydrology file to the name of the respective *.prl file
3	Execute simulation
4	After simulation has completed delete pre-run hydrology file

## 6 Evaluation of a completed run

To evaluate a simulation select the respective *output directory* in the FROGS.exe tool and push *Evaluate* button. *Substance*, *Main Crop*, and *Application Scheme* are not relevant for results evaluation.

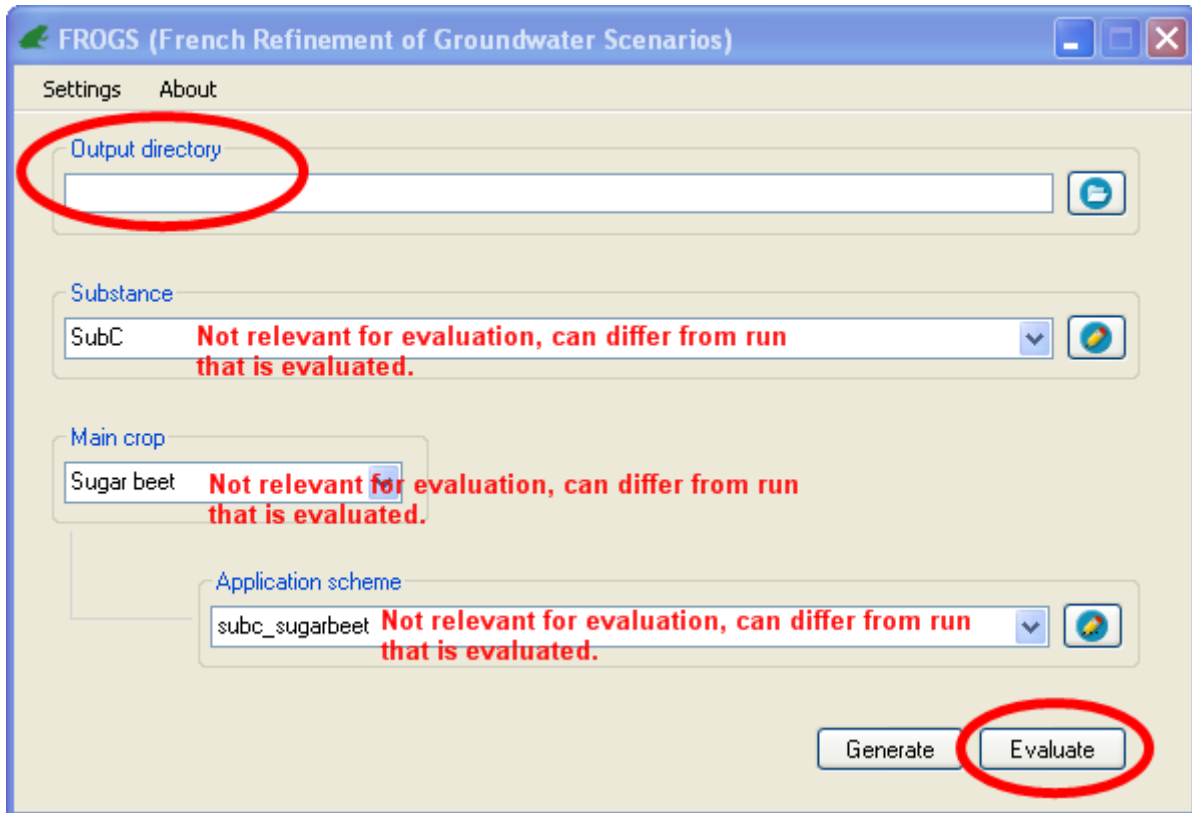


Figure 23 Evaluate completed FROGS run

The selected output directory should contain at least all the *\*.sum files* **and** "*catalogue.txt*" in order to be able to assign each Run-ID to a specific scenario.

After successful evaluation the following files will be created in the output directory:

- FROGS Cumulative Areal distribution - MET-C.png
- FROGS Cumulative Areal distribution - MET-C.txt
- FROGS Cumulative Areal distribution - SubC.png
- FROGS Cumulative Areal distribution - SubC.txt
- FROGS Summary.txt

Figure 24 Files generated during evaluation of a completed run

**Table 6 Definition of files generated during evaluation of a completed run**

<b>File</b>	<b>Definition</b>
FROGS Summary.txt	Each line represents the 80 <sup>th</sup> percentile PEC <sub>gw</sub> for a scenario (AU-Soil-Crop) and a substance
FROGS Cumulative Areal distribution - xxx.png	"self-explanatory" from file name
FROGS Cumulative Areal distribution - xxx.txt	Raw file for "FROGS Cumulative Areal distribution" plots  Algorithm for derivation from "FROGS Summary.txt for one substance: <ul style="list-style-type: none"><li>• Sort PEC<sub>gw</sub> in ascending order</li><li>• Accumulate areas (AU-Soil-Crop-area)</li><li>• Normalize accumulated areas to 0 ... 1 (e.g. specific AU-Soil-Crop-area divided by total area)</li></ul>