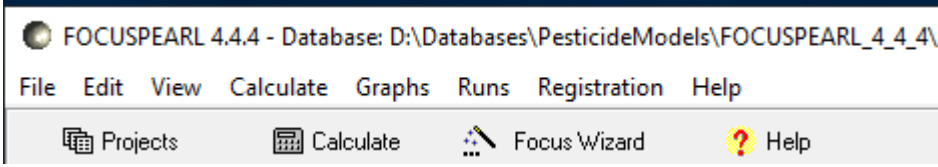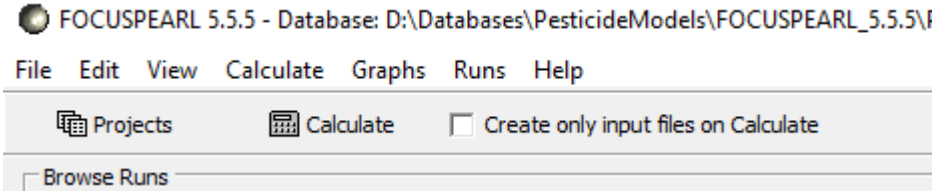# Procedure for archiving modelling results for dossier submissions

In the tables below a short description is presented of the procedure to be followed in order to archive the results from a calculation of a certain application. This procedure is designed to archive all necessary files in order to be able to reconstruct the calculations performed on a later point in time. The procedure to reconstruct an archived calculation is not described here as this is basically the reverse process.

Summarizing the process of archiving calculations follows these steps (detailed description for each application is presented in the table below):
- Copy the required files to a compressed folder (i.e. zip-file);
- Rename the zip-file according to the following format:
  <applicant's name>_<active substance>_<model>_<version number of model>.zip
- Upload the zip-file to the Ctgb dossier submission system

Please note that Ctgb has indicated the default directory for the model databases, input and output files, that is used by the application during installation. This default directory might differ from the directory chosen during the installation by your organisation. For some applications the location of the directory of the database and projects can be retrieved from within the GUI. For these applications this has been indicated in the table below.

application	Version	procedure
CAKE	3.3	CAKE study files (*.csf) and reports (*.rtf) are saved to a directory chosen by the user. These files need to be archived.
ESCAPE	2	Output files *.rtf files in the folder "D:\Escape.2\output". Input files (*.chn, *.apn, *.scn) located in the folder "D:\Escape.2\intput". If the user does not change the name than these files will be named " Programcheck.*" which is the default example simulation.
FOCUS PEARL	4.4.4	Copy the following files and folders to a Winzip-file: • The whole folder "PearlDB" • The file "PearlDB.fdb" The location is indicated in the title bar of the application: FOCUSPEARL 4.4.4 - Database: D:\Databases\PesticideModels\FOCUSPEARL_4_4_4\ File Edit View Calculate Graphs Runs Registration Help Projects Calculate Focus Wizard Help
FOCUS PEARL	5.5.5	Copy the following files and folders to a Winzip-file: • The whole folder "PearlDB" • The file "PearlDB.ib" • SPIN database "spin_db.fdb" The location of the PEARL folder and database file is indicated in the title bar of the application: FOCUSPEARL 5.5.5 - Database: D:\Databases\PesticideModels\FOCUSPEARL_5.5.5\ File Edit View Calculate Graphs Runs Help Projects Calculate ☐ Create only input files on Calculate Browse Runs The location of the SPIN database can be displayed within the GUI of SPIN, by selecting "Help" in the menu bar and select "About SPIN":

		SPIN (Substances Plug IN) 3.3 GUI Version: **v.3 (internal version 1.4.3)** Database Version: **v.3 (internal version 68)** Date: **12/6/2018** Design / construction: **Daniel van Kraalingen,** **Johnny te Roller** **(Alterra, Earth Informatics)** Path to dll: **D:\Program Files (x86)\PesticideModels\SPIN\Bin\spin_dll.dll** Path to database: **D:\Databases\PesticideModels\SPIN\spin_db.fdb**

FOCUS PELMO	6.6.4	Copy the following files and folders to a Winzip-file:
		• The file substance file created by the user "<name>.psm" from the default directory
		  default directory: *C:\FOCUS_PELMO.664*
		• The whole folder "<name>.run" from the directory
		  default directory: *C:\FOCUS_PELMO.664\FOCUS*

FOCUS PRZM_GW	4.6.2	After the calculations new project(s) need to be archived along with the PRZM_GW database. In the directory structure of PRZM_GW there is a default location *C:\FGRAT\PROJECTS.* If this folder is selected all input and output files will be written to this folder. Alternatively a new folder can be created within this default directory. Copy the following files and folders to a Winzip-file: • The whole projects folder from the directory chosen by the user • The files "chmdat.dat" and "chmnum.dat" from the directory *C:\FGRAT\wpic*

FOCUS SWASH	5.3	After the calculations new project(s) need to be archived along with the SWASH and SPIN database.
		
		Copy the following files and folders to a Winzip-file:
		• relevant project folders from the directory:
		  default directory *C:\SwashProjects*
		  make sure to copy the whole project folder including all files and subfolders

		• SWASH database "SWASH.fdb" from the directory:
		default directory: C:\SWASH\Data
		• SPIN database "spin_db.fdb"
		
		The location of the SPIN database can be displayed within the GUI of SPIN, by selecting "Help" in the menu bar and select "About SPIN":
		
		SPIN (Substances Plug IN) 3.3
		
		GUI Version: v.3 (internal version 1.4.3)
		Database Version: v.3 (internal version 68)
		Date: 12/6/2018
		Design / construction: Daniel van Kraalingen,
		    Johnny te Roller
		    (Alterra, Earth Informatics)
		
		Path to dll: D:\Program Files (x86)\PesticideModels\SPIN\Bin\spin_dll.dll
		Path to database: D:\Databases\PesticideModels\SPIN\spin_db.fdb

GEM	3.3.2	After the calculations new project(s) need to be archived along with the SWASH and SPIN database. Copy the following files and folders to a Winzip-file: • The whole folder "Projects" from the default directory: C:\Users\<username>\Documents\PesticideModels\GEM\Projects • The whole folder "Database" from the directory: C:\Users\<username>\Documents\PesticideModels\GEM\Database • SPIN database "spin_db.fdb" The location of the SPIN database can be displayed within the GUI of SPIN, by selecting "Help" in the menu bar and select "About SPIN":

SPIN (Substances Plug IN) 3.3

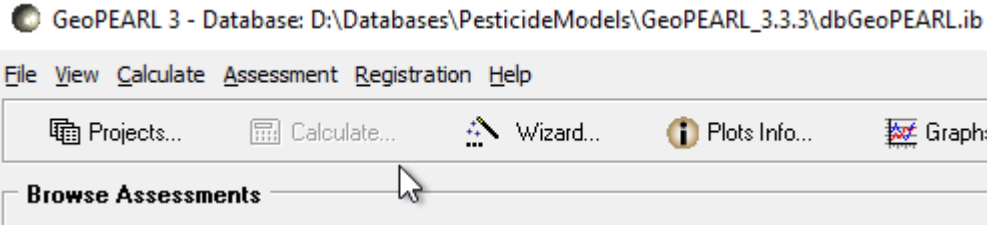|	
GUI Version:	**v.3 (internal version 1.4.3)**
Database Version:	**v.3 (internal version 68)**
Date:	**12/6/2018**
Design / construction:	**Daniel van Kraalingen, Johnny te Roller (Alterra, Earth Informatics)**
Path to dll:	**D:\Program Files (x86)\PesticideModels\SPIN\Bin\spin_dll.dll**
Path to database:	**D:\Databases\PesticideModels\SPIN\spin_db.fdb**

		If SAFE_SL was used to perform multiple soilless assessments, then these assessments are also archived via the above described procedure. SAFE_SL creates a subdirectory named "SCENARIOS" in the GEM projects folder that was used as a basis for the assessment. If SAFE_SB was used, then output is written to a user specified output path. This folder needs to be archived separately (see below).
SAFE_SB	1.1	Output is written to a user specified output path. Copy this folder to a Winzip-file.
SAFE_SL		Assessments are archived via the procedure described for GEM. SAFE_SL creates a subdirectory named "SCENARIOS" in the GEM projects folder that was used as a basis for the assessment.
GeoPEARL	3.3.3	Copy the following file to a Winzip-file: • The file "dbGeoPEARL.ib" The location of the GeoPEARL database file is indicated in the title bar of the application:

		![GeoPEARL 3 screenshot] GeoPEARL 3 - Database: D:\Databases\PesticideModels\GeoPEARL_3.3.3\dbGeoPEARL.ib File View Calculate Assessment Registration Help 📇 Projects... 📠 Calculate... ✎ Wizard... ⓘ Plots Info... 📈 Graph: **Browse Assessments**
KinGUI	2.1	After the calculations the R-script and the results need to be archived. All relevant files are located in the trial folder which needs to be specified by the user. In the directory structure of KinGUI there is a default working directory *C:\KinGUII\WorkingDirectory* in which trial folders can be created. Copy the following folders to a Winzip-file: • All relevant trial folders from the directory specified by the user: e.g. *C:\ KinGUII_2.1\WorkingDirectory\< user >*
Steps1-2 in FOCUS	3.2	After the calculations substance data and results need to be archived. Please note that the results can also be transferred to your own desktop using the clipboard. For the diagrams created by Steps1-2 the "Copy to clipboard" button works correctly. However, for the report it does not. You have to manually select the relevant text from the report and use Ctrl + C to copy the content to the clipboard. Copy the following files and folders to a Winzip-file: • Steps1-2 database "pesticide.txt" from the default directory *C:\Steps.12* • The whole folder "results" from the default directory *C:\Steps.12*
SWAN	5.0.1	After the calculations new project(s) need to be archived. SWAN creates new TOXSWA input files, based on an existing valid SWASH Project applying the selected mitigation. After the calculation, new TOXSWA output files are created. Both input and output files are saved to a directory specified by the user for the SWAN project. See below for the criteria for a valid SWASH Project and the conditions for the SWAN project. In order to be a valid SWASH FOCUS project, the following conditions on the source SWASH project folder must be met: • The project folder must exist • The project folder must contain a MACRO folder

		• The project folder must contain a PRZM folder • The project folder must contain a TOXSWA folder • There must be at least one .TXW file in the TOXSWA folder • For each .TXW file, there must be a corresponding .M2T or .P2T file • The files within the project folder must relate to exactly one substance • The files within the project folder must relate to exactly one crop The following conditions on the SWAN output project folder must be met: • The output folder must exist • The output folder must be different from the source project folder • The output folder must not contain MACRO, PRZM or TOXSWA folders Copy the following folders to a Winzip-file: • All relevant trial SWAN project folder from the directory specified by the user
TOXSWA	1.2	After the calculation, substance data, scenario data and the output files need to be archived. Copy the following files and folders to a Winzip-file: • The folder of the scenario created by the user from the directory *C:\TOXSWA\Scenarios* • The folder of the substance created by the user from the directory *C:\TOXSWA\Pesticides* • The folder with the name "<scenario> + <substance>" from the directory *C:\TOXSWA\RUNS*