USER MANUAL OF THE FOCUS PRZM SHELL

"FOCUS PRZM GROUNDWATER TOOL"

Version 2.0, February 2011

Introduction

The development of revised scenarios by the FOCUS Ground Water group resulted in the need for software changes to both the model and the shell in order to use the PRZM (**P**ESTICIDE **R**OOT **Z**ONE **M**ODEL) for assessing potential to move to ground water as part of the EU registration procedure. While the operation of the shell seems quite similar to the previous versions, there were a number of changes to the model and as well as to the scenarios.

The underlying model is the executable WINPRZM.EXE. This is a truly *Windows* based program, independent from any DOS limitations, written in FORTRAN and suitable for use of 32 and 64 bit machines. A windows shell called FGRAT.EXE (**F**OCUS PRZM **Gr**ound W**a**ter **T**ool) was built around the PRZM executable. Included in FGRAT is a tool for preparing graphs and tables of results for visualizing and reporting of model results. The major objective was to make the creation of PRZM input files easier and to fulfil the FOCUS Tier 1 requirements for European groundwater assessments. Further details about FOCUS and the implementation of the Council Directive 91/414/EEC can be found at http://focus.jrc.ec.europa.eu/. The program coding was conducted by Waterborne Environmental (http://www.waterborne-env.com/) in close co-operation with the FOCUS PRZM development team. The FOCUS PRZM shell is optimised for a screen resolution of 1024x768 pixel and provides the following features:

- user-friendly scenario and parameter definitions in a *Microsoft Windows* environment.
- pre-definition of the European FOCUS Tier 1 groundwater scenarios.
- modified and enhanced WINPRZM code (Version 4.51).

A detailed description of the process and scenario parameterisation in the generated PRZM input files is given in the "FOCUS PRZM Parameterisation Document" provided with the installation files. Additional information about FOCUS groundwater assessments and the models used can be found at the FOCUS webpage http://focus.jrc.ec.europa.eu/gw/index.html.

Data files and scenario definition

The information necessary to run WINPRZM.EXE is divided into a number of input data files:

- parameter file including the scenario definition *.inp
- climate file providing the weather data used *.met
- file with definition of the PRZM run options *.run

The shell FGRAT.EXE allows the creation of the required input files by the user. All scenario compound and application specific information is also stored in the Master Project File called “master.fpj”. In addition a file of the type *.scn is created in order to support the grapher of the PRZM shell with necessary information for the data analysis and data visualisation. It should be noted that the FOCUS PRZM 3.5.2 parameter and weather files are not compatible with older PRZM versions.

The scenario and parameter definitions are based on the **USER INPUT** (Input to be specified by the user in the FOCUS PRZM shell), on **FOCUS DEFINITIONS** (Definitions made by the FOCUS working group) and **DEVELOPMENT DEFINITIONS** (Definitions made during the FOCUS PRZM shell development). Parameter definitions based on **FOCUS** or **DEVELOPMENT DEFINITION** are not changeable by the user in the FOCUS PRZM shell. Some input definitions are automatically specified as **FOCUS SCENARIO SPECIFIC** based on the **USER INPUT** according to a selection of predefined values based on **FOCUS** or **DEVELOPMENT DEFINITIONS**. All predefined and generated data files provided by the FOCUS PRZM shell may be changed manually to realise special scenario definitions. None of these shell-generated data files should be modified under any circumstances for standard FOCUS TIER 1 simulations!

After a completed simulation run the relevant scenario output data is given in six ASCII files of the type *.ann, *.hyd, *.cnc, *.msb, *.out and *.zts. The shell will analyse those files automatically and provide the user with result tables and graphics, as required from FOCUS. For FOCUS TIER 1 runs the user doesn't need to analyse the output files in a different way. But the grapher of the PRZM shell also allows to export results for each simulated scenario in an ASCII file of the type *.tab. These files may be used for further data analysis as they include all output data required for FOCUS based Tier 1 calculations. All other files must not be used for standard FOCUS Tier 1 risk assessments!

Getting the shell installed and started

The FOCUS PRZM shell can be installed on any standard IBM compatible PC with a Windows (95, XP, VISTA, WIN7) compatible operation systems. To install the shell the user should follow the instructions given during the set-up procedure. All required files will be installed automatically in the default the installation path C:\FGRAT\. The PRZM shell requires 50 MB hard disk space for the installation plus additional 50 MB for temporary files.

In very few cases it may be necessary to adjust the automatic installation by the following amendment:

- The ASCII file “Pfdrv.ini” created during the installation in the directory C:\FGRAT\ is also required in the directory C:\WINDOWS\ (this path is fixed and NOT depending on the *Windows* installation). The file “pfdrv.ini” contains only two lines, one with the drive letter of the Windows drive (e.g. C:) and another with the drive letter of the CDROM (e.g. G:). The drive letters may be adjusted manually.

After a successful installation the shell can be started by double clicking on FGRAT.EXE or by starting any shortcut “FPGWT” to the executable. The starting screen should appear including a picture of well monitoring equipment in a field. The starting window of the PRZM shell is given together with some explanations in Figure 1.

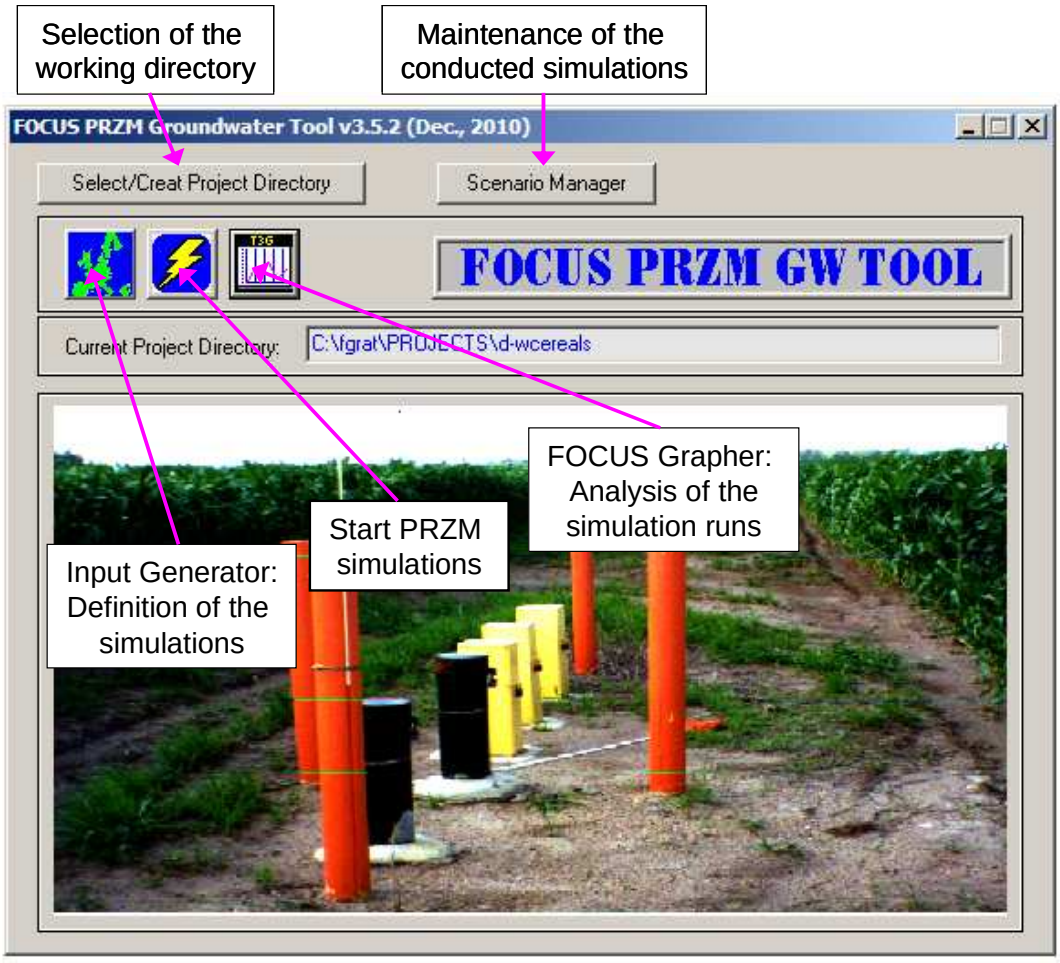


Figure 1. The starting screen of the FOCUS PRZM shell before definition of a project directory.

Project Directory and the Master Project File

Directly after the start of FGRAT the user has to specify the active project directory. This is necessary to create with the shell the pesticide input data files for WINPRZM. All relevant

input/output data of a simulation run is saved under this working directory. Therefore FGRAT needs to have full read/write permission for the specified directory. New directories can be created on hard disks or network drives using the shell, *Windows Explorer* or other tools. Long filenames are possible. A standard working directory to be automatically used as default directly after start of FGAT, e.g. C:\FGRAT\FOCUS\PROJECTS, may be defined in the first line of the file "startdir.ini" located in C:\FGRAT. The default directory just after installation of FGRAT is not defined or "unset". Note that only one directory level can be created at one time when specifying the project directory. For example, one cannot create the file C:\FGRAT\FOCUS\PROJECTS\PesticideD\apples in one step while in the Select/Create Project Directory portion of the shell. However, this could be done by specifying the directory C:\FGRAT\FOCUS\PROJECTS\PesticideD, exiting and re-entering the Select/Create Project Directory, chosing C:\FGRAT\FOCUS\PROJECTS\PesticideD and then typing \apples. Another option would be to create multi-level files outside the PRZM shell. However, one would still need to select the directory within the PRZM shell.

The user should use the option to switch between different scenarios by choosing different working directories. Each simulation scenario may be re-run and re-analysed later on by choosing the specific project directory. The shell guarantees that only valid FOCUS crop/soil combinations and appropriate input scenarios can be selected (e.g. multiple scenario runs of 2 or more FOCUS locations). It is guaranteed that each standard FOCUS TIER 1 single or multiple simulation scenario can be only done in its own individual project directory!

The FOCUS PRZM shell generates a Master Project File (MPF). This file named "MASTER.FPJ" contains all scenario specific information necessary to characterise the entire simulation project in the selected working directory. After the user has specified an active project directory the shell directly checks if a MPF is existing in this directory. If yes the shell returns an output window as given in Figure 2 asking for the further procedure. The user may decide between one of these options to use the MPF.

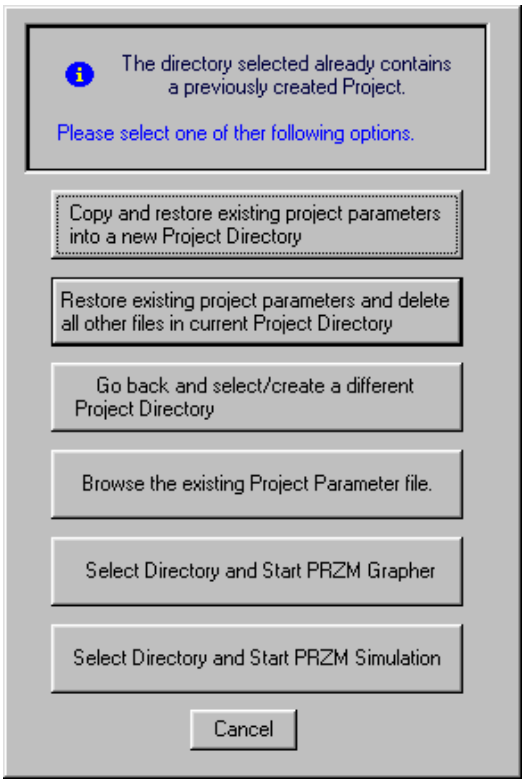


Figure 2. FOCUS PRZM shell giving different options to use of the Master Project File.

Note that the Master Project File contains **all** parameter information necessary to characterise a complete FOCUS run. The MPF can be easily used to exchange FOCUS simulation scenarios between different persons or bodies involved. A MPF from a different source needs only to be copied to a path valid to be used as active working directory. By employing the MPF it is possible to validate and re-create each scenario, compound and application specific model input used to generate a particular FOCUS scenario.

Format of the Master Project File

The definition of the scenario, compound and application specific parameters is done corresponding to the formats used in the PRZM parameter file (*.inp). A typical example for a Master Project File is given below in Figure 3. The depicted Master Project File was created for for a parent compound with one metabolite applied two times each season, with a different application rate for the first and second application.

```
 1 Project File Created: 2010-12-10,  16:30:23
 2 FOCUS PRZM Groundwater Tool v3.5.2 (Dec., 2010)         WINPRZM4.51
 3 Parent Compound: FOCUS dummy C                      Crop: Cereals (Winter)
 4
 5 CROP           :  7 1
 6 SCENARIO       : 111111111
 7 ROTATION       : 1
 8 RELATIONSHIP   : 2
 9 CHEMICAL       : 2 0010101
10  Chemical Name: FOCUS dummy C       Metab. dummy C
11   Molecular Wgt:    200.000   150.000
12   Plant Upt Fct:      0.500     0.500
13   Part Cff Mth :          1         1
14   Part Cff Fct :    172.000    52.000
15   Freund Exp   :      0.900     0.900
16   Vapor Pres   : 0.1000E-060.1000E-06
17   Solubility   : 0.5000E+020.9000E+02
18   Degr. PH1    :     20.000   100.000
19   Degr. PH2    :      0.000     0.000
20   % Degr. PH1  :     71.000     0.000     0.000
21   % Degr. PH2  :      0.000     0.000     0.000
22   Bi-Phase     :          0         1
23   Q10 FAC      :      2.580     2.580
24   Q10 Temp     :     20.000    20.000
25   Moisture Exp :      0.700     0.700
26   Moisture Cnt :    100.000   100.000
27   Moisture Type:          2         2         2      -999
28   Foliar 1/2   :      0.000     0.000
29   Foliar Wash. :      0.000     0.000
30 APPLICATION    : 222
31   Days Rel     :         -1        10
32   Day          :         -1        10
33   Month        :          0         0
34   CAM          :          1         1
35   Depi         :      4.000     4.000
36   Rate         :     1.0000    5.0000
37   Drift        :      0.000     0.000
38   Eff          :    100.000   100.000
```

Figure 3. Example of the Master Project File (parent with one metabolite, blue numbers added).

The information included in the Master Project File is complete but minimised with regard to the FOCUS default settings. Information about metabolites, ageing factors or modified bio-degradation factors are only included if relevant. Following information is coded in the individual lines of the Master Project File:

Line 1: Date on which the file was created by the FOCUS PRZM shell.

Line 2: Version of the FOCUS PRZM Shell & PRZM version

Line 3: Name of the parent compound & crop used

Line 4: empty line

Line 5: Internal index of the used crop (7 = winter cereals) and runoff switch (1 = no runoff)

Line 6: Index used scenarios (1 = used; 0 = not used for the simulation run) scenarios are coded in following standard order: CHJKNPOST

Line 7: Crop Rotation (1 = no crop rotation, 26 year met file)

Line 8: Relationship between parent and metabolites (2 = parent with one metabolite)

Line 9: Chemical Index & activated model processes

Line 10-29: Chemical properties (parent and metabolites)
Line 30-38: Application scenario (here four application relative to emergence)
Line 39-57: Modified soil bio-degradation factors separated between parent and metabolites (-999.00 = soil layer not used for this soil scenario)
Line 58-61: Ageing factors and non-equilibrium sorption parameters for parent and metabolites (see later discussion)
Line 62: empty line

Scenario Manager

The “Scenario Manager” allows the maintenance of conducted FOCUS scenarios. The user can enter for each conducted scenario an identifier or short help text as annotation. It is also possible to delete individual project directories.

Creating the data files for a PRZM simulation

To start the scenario definition and to enter the necessary pesticide input data the user has to click on the icon "Scenario Generator" of the PRZM shell. The input generator (Figure 4) allows the specification of the necessary input data in four steps:

1) Selection of one of the predefined location and crop specific scenarios and activation of some major processes like foliar application, bi-phasic degradation or aged sorption.

2) Definition of the compound specific physical-chemical and efate properties. A separate efate screen is used for parent and each metabolite (max. two).

3) Definition of the compound application scenario.

4) Creation of the input files in the specified working directory (“Write”).

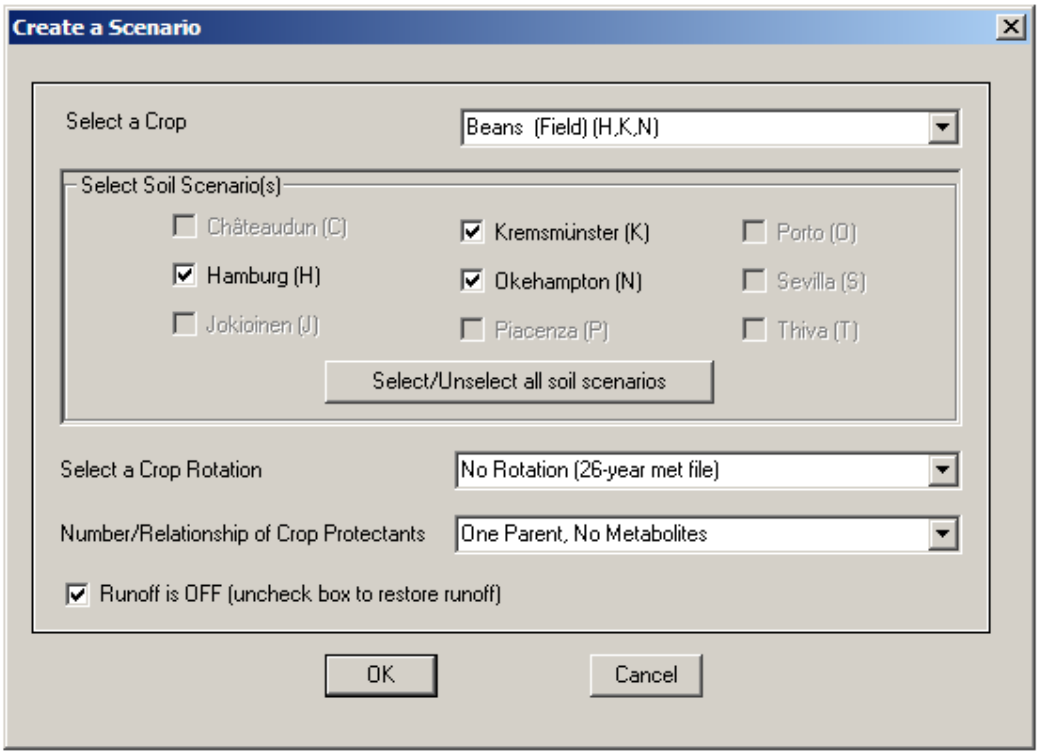


Figure 4. FOCUS PRZM Input Generator with selected scenario window.

All the functions of the FOCUS PRZM Input Generator can be selected simply by clicking on the specific menu points. The scenario, efate and application windows should be closed by clicking on OK. All four input steps should be completed in the given consecutive order (Scenario, Efate, Application, Write) to allow everything to work fine!

The user of the PRZM shell is expected to be familiar with the use of simulation models for environmental risk assessments in general. The creation of the input files should be then self-explainable. For FOCUS Tier 1 simulations the user has to make sure that the process implementation and parameter definition is done according to the FOCUS guideline and the intended use of the compound.

For the most part the metabolite properties can be defined independently from the parent properties (e.g. Freundlich, volatilisation, temperature and moisture corrected degradation, bi-phasic degradation). The bio-degradation factors of a metabolite are handled in the parent check box as an independent data set.

All compound specific parameters (parent and metabolites) can be saved in a chemical database provided with the shell. This allows the use of the same compound parameters for additional simulations of different soil and crop scenarios. However, note that the non-equilibrium sorption parameters are not saved with the chemical properties. It is possible to

maintain the database and to delete single entries. The whole database may be also deleted manually by starting the batch file CHM.BAT found in the directory C:\FGRAT\WPIC.

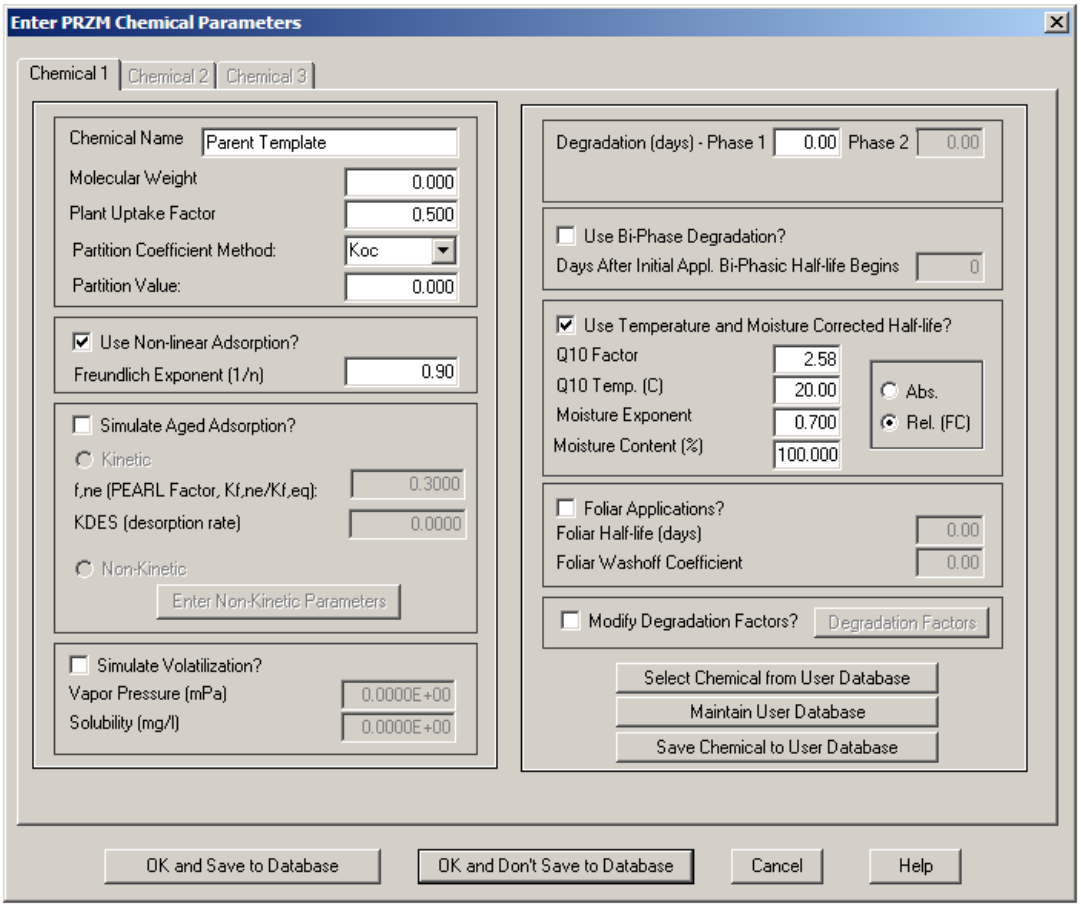


Figure 5. Definition of the chemical parameters (here chemical 1 = parent).

After all scenario, efate and application data has been specified, the input files have to be written in the project directory by clicking on the "Write" button. A click on “Exit” will close the FOCUS PRZM Input Generator and will return to the FGRAT starting screen.

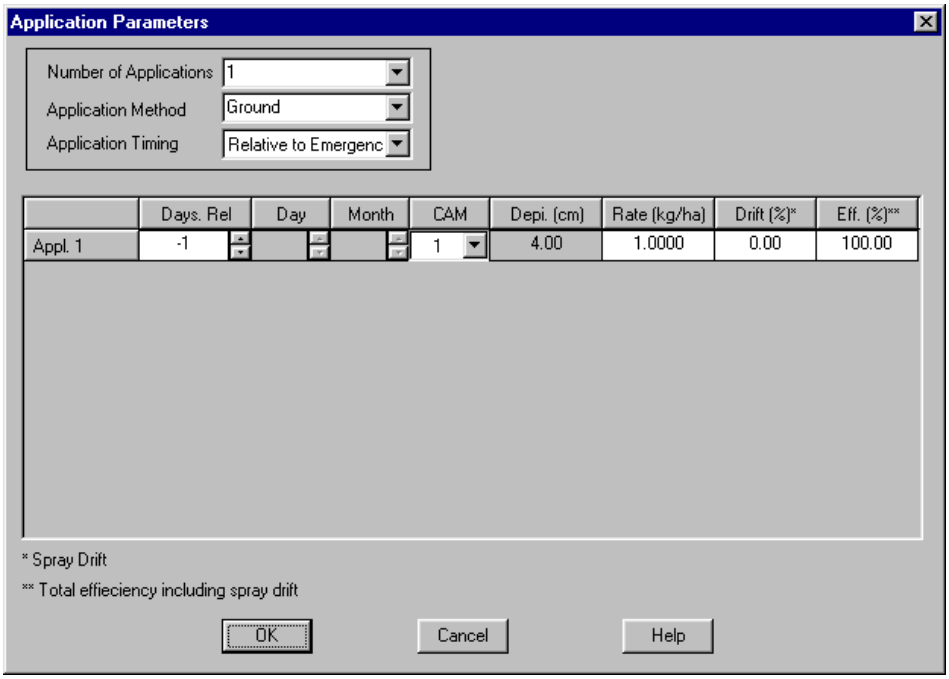


Figure 6. Definition of the application parameters.

Handling of degradation rates in PRZM and in the PRZM shell

For ease in specifying degradation rates, the degradation kinetics is specified in the new WINPRZM differently than in the former DOS versions of PRZM. A typical input window of the metabolite parameters is given in Figure. 7.

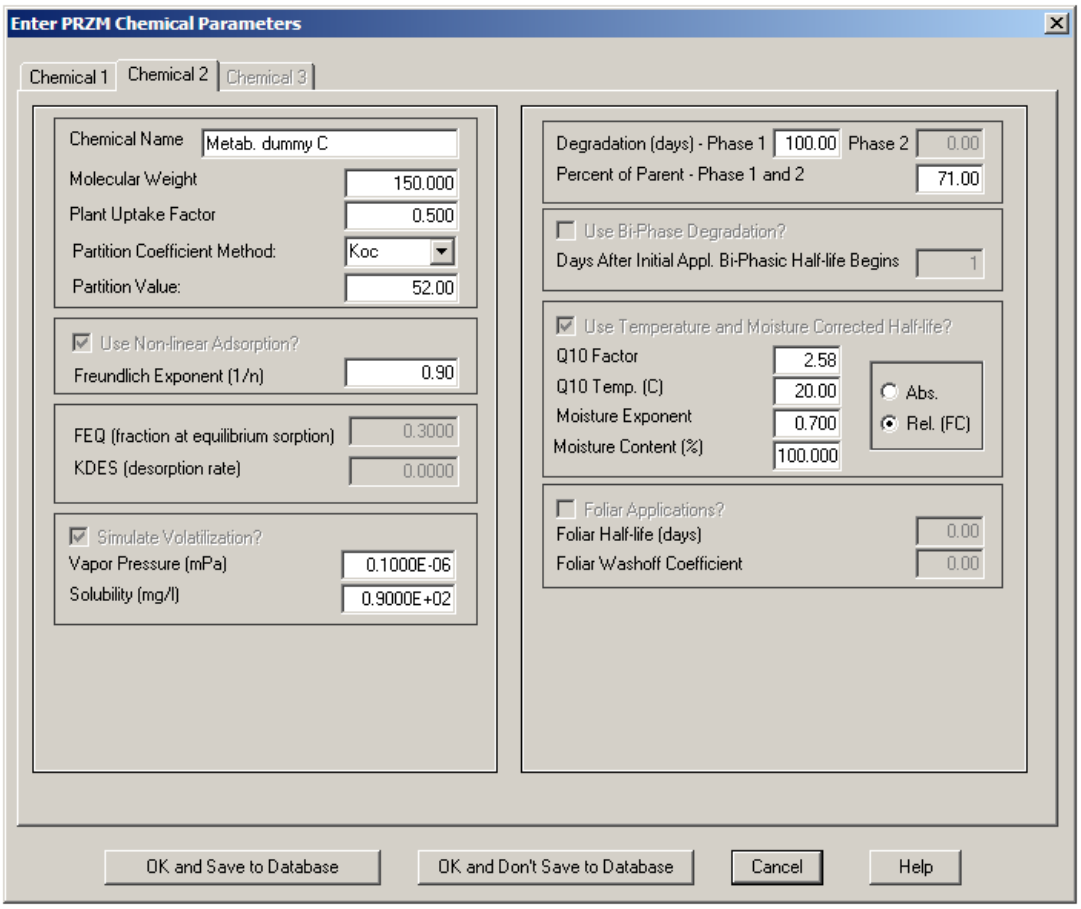


Figure 7. Input window to define the metabolite parameters (here chemical 2).

In contrast to the definition of the metabolisation parameters given in the PRZM 3.0 manual some major changes apply in WINPRZM. Details are explained in the FOCUS PRZM parameterisation document. The PRZM shell will automatically do the necessary calculations to produce the parameters as required in the WINPRZM input file according to the USER INPUT.

Each compound to be used in the simulation scenario must be characterised by the total first order degradation half-life (regardless of whether the dissipation is to a specified or unspecified metabolite, to CO_2 or to bound residues) (see Figure 5 and Figure 7). In addition to this the formation percentage (in the FOCUS report also called “transformation fraction”) going from the parent to a metabolite or from one metabolite to another has to be defined for each metabolite used in the simulation (see Figure 7: “Percent of Parent”). The shell automatically uses the affiliated molecular weights to adjust the PRZM input formation fraction by the molecular weight relation. In doing so the correct mass flow and output concentrations are guaranteed.

Non-equilibrium sorption

The implementation of non-equilibrium sorption in PRZM has been discussed in a companion document included in the installation package of FOCUS PRZM 3.5.2.

The FOCUS PRZM shell was modified to process the additional parameter necessary to consider kinetic sorption. In addition the old PRZM option using non-kinetic “aged” sorption factors is available to be consistent with previous versions of PRZM.

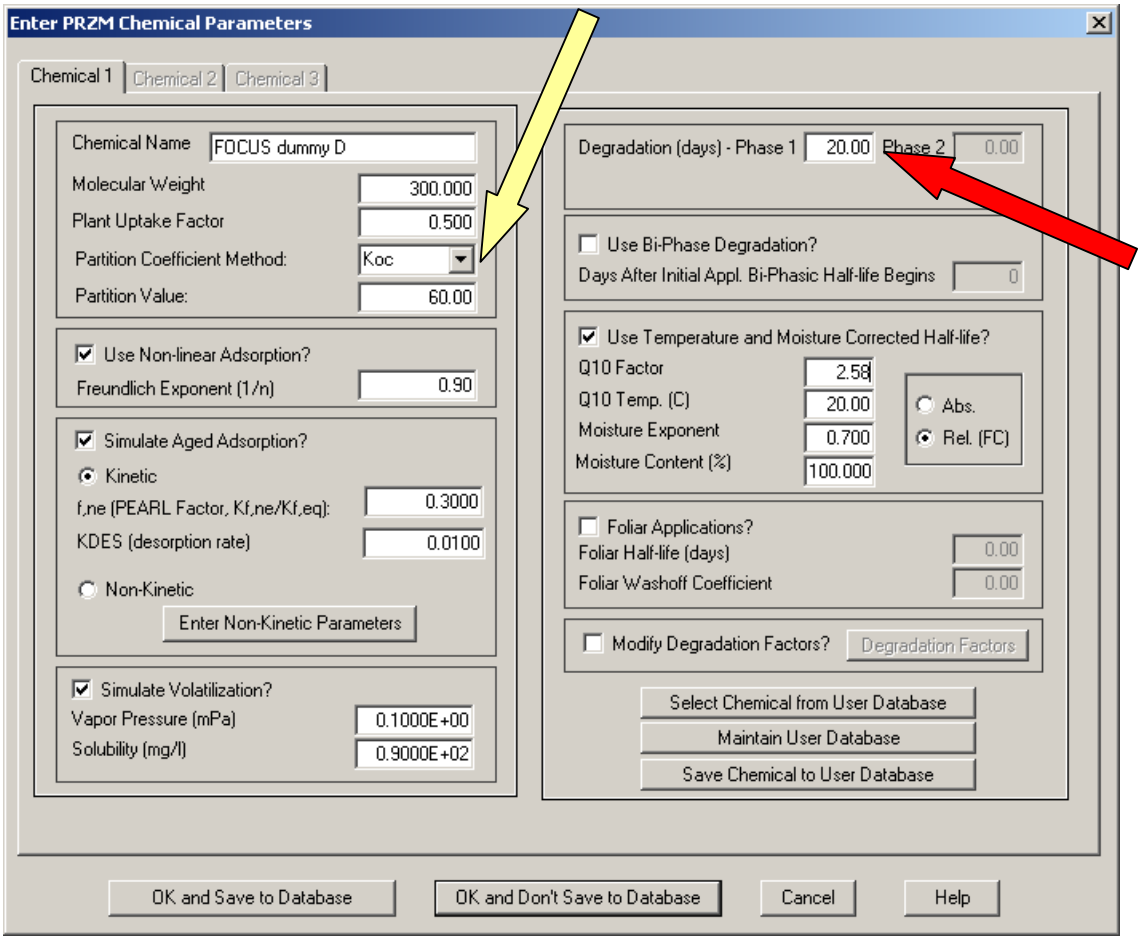


Figure 8. Extended input sheet to consider kinetic sorption in PRZM.

In the field “Partition Value - Koc” (see the yellow arrow in Figure 8) always the (normal) equilibrium sorption Koc value related to the whole soil has to be entered (consistent with previous versions of PRZM).

In the field “Degradation” (see the red arrow in Figure 8) the adjusted degradation DT50 of the equilibrium phase (which is always shorter then the degradation DT50 of the total bulk soil) has to be entered (consistent with the PEARL). This is applicable to both DT50 values

in the case bi-phasic degradation is simulated. The adjusted degradation DT50 of the equilibrium phase may be estimated based on the relation given in the following equation:

$$DT50_{eq} = \frac{DT50_{tot}}{1 + f_{ne}}$$

Kinetic sorption parameters are saved in the PRZM Master Project File "master.fpj" (see the example in Figure 9). Consistent with previous versions of PRZM the Master Project File summarised all relevant information to re-generate a simulation a run. Regardless whether 1, 2, or 3 compounds are being simulated, there is always three lines of sorption parameters in the Master Project File.

```
    Project File Created: 2009- 9-16,  16:11:37
FOCUS PRZM Groundwater Tool v3.5.2 (Oct., 2008)         PRZM4.51
Parent Compound: FOCUS dummy D                      Crop: Cereals (Winter)

CROP            :  7 1
SCENARIO        : 010000000
ROTATION        : 1
RELATIONSHIP    : 1
CHEMICAL        : 1 0010111
  Chemical Name: FOCUS dummy D
  Molecular Wgt:    300.000
  Plant Upt Fct:      0.500
  Part Cff Mth :          1
  Part Cff Fct :     60.000
  Freund Exp   :      0.900
  Vapor Pres   : 0.1000E+00
  Solubility   : 0.9000E+02
  Degr. PH1    :     20.000
  Degr. PH2    :      0.000
  % Degr. PH1  :      0.000     0.000     0.000
  % Degr. PH2  :      0.000     0.000     0.000
  Bi-Phase     :          0
  Q10 FAC      :      2.580
  Q10 Temp     :     20.000
  Moisture Exp :      0.700
  Moisture Cnt :    100.000
  Moisture Type:          2         2         2         1
  Foliar 1/2   :      0.000
  Foliar Wash. :      0.000
APPLICATION     : 122
  Days Rel     :         -1
  Day          :         -1
  Month        :          0
  CAM          :          1
  Depi         :      4.000
  Rate         :     1.0000
  Drift        :      0.000
  Eff          :    100.000
AGING FACTORS   :
  CHemical 1   :          0         0         0         0         0    1.0000
1.0000    1.0000    1.0000    1.0000    0.3000    0.0100
  CHemical 2   :          0         0         0         0         0    1.0000
1.0000    1.0000    1.0000    1.0000    0.3000    0.0000
  CHemical 3   :          0         0         0         0         0    1.0000
1.0000    1.0000    1.0000    1.0000    0.3000    0.0000
```

Figure 9. Master project file with kinetic sorption parameters marked in blue.

Starting the PRZM simulation

To start the PRZM32 simulation run of the defined scenario simply click on the "Run PRZM" button. Then the shell will automatically start the executable WINPRZM.EXE. During the simulation run the PRZM shell is not able to conduct other actions. It is impossible to run two simulations at the same time. The user may relax during the waiting time or work with other *Windows* applications. An example for a typical output window during a simulation run of PRZM is given in Figure 10.

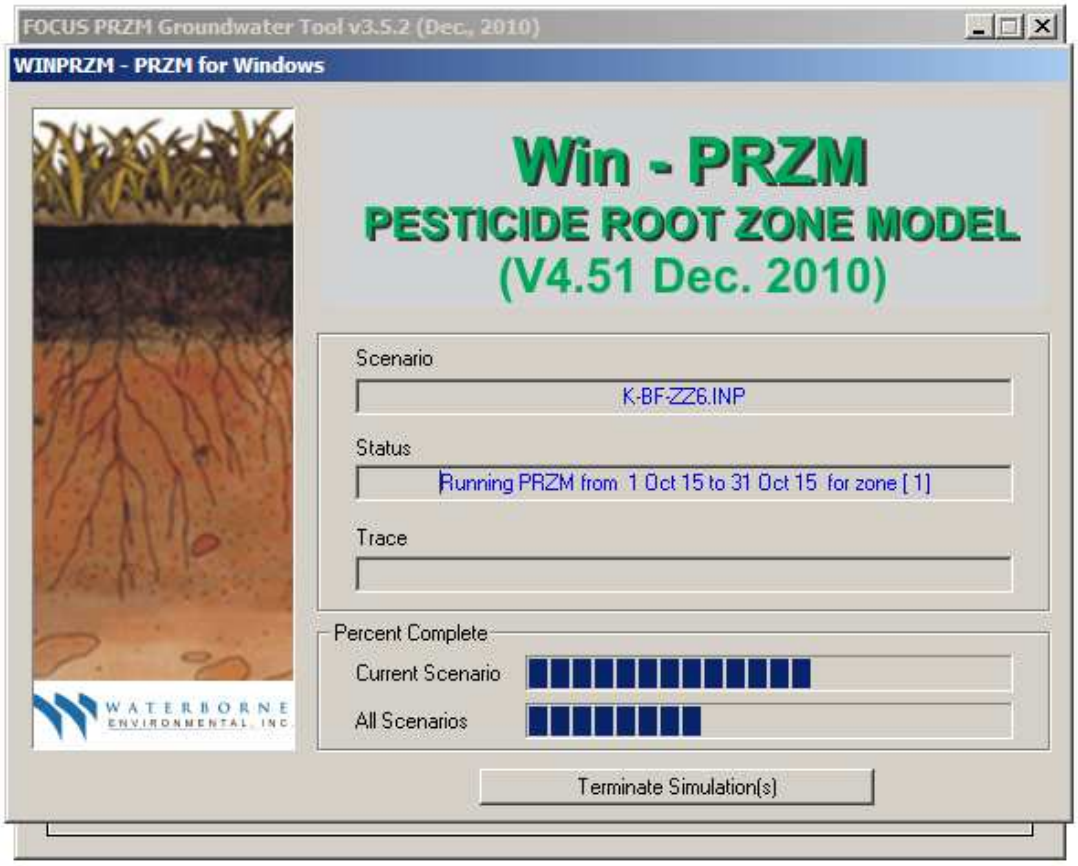


Figure 10. Output window during a PRZM32 simulation using WINPRZM.EXE.

Evaluation of the PRZM simulation

After the PRZM simulation has been finished (output window has been automatically closed) the user may wish to evaluate the results of the conducted simulation with the FOCUS PRZM Grapher provided with the shell. Clicking on the “FOCUS Grapher” button will start the grapher and automatically generate *.tab files including all data required for the FOCUS Tier 1 risk assessment. The detailed simulation results of a selected location scenario and the 80th percentile data can be analysed. The results can be directly visualised with the FOCUS PRZM Grapher as tables or as graphics. All figures can be exported as *Windows Meta Files* or ASCII files or printed directly. To do so, simple select the table or graphic and click on “Print” or “Export” respectively. The *.tab files may be also used for easy reporting or for a

further non-standard data analysis. A short summary of the 80th percentile concentrations is also generated in a file named “CNC-80.ANN”. This file also contains selected values for the water balance averaged over the 20 year simulation period (40 or 60 for every applications made every second or third year).

Examples for a typical shell output are given in Figures 11 – 16 on the next pages. The shell provides according to the FOCUS requirements a collection of different evaluation types:

- Groundwater concentration at 1 m
- Groundwater concentration at core depth
- Mass balance at 1 m
- Mass balance at core depth
- Hydrology summary (1 m and core depth)
- Summary of 80th percentile leaching concentrations at 1 m

All generated graphics, tables and output files are clearly marked with the version number of the PRZM shell used. The version “FOCUS PRZM Groundwater Tool v3.5.2 (December, 2010)” has been used to generate the output used in this manual. Please check the FOCUS webpage for the most recent version of the FOCUS PRZM shell.

Program exit

Exit the FOCUS PRZM Ground Water Assessment Tool by clicking on the **x** button in the upper right hand corner of the starting screen.

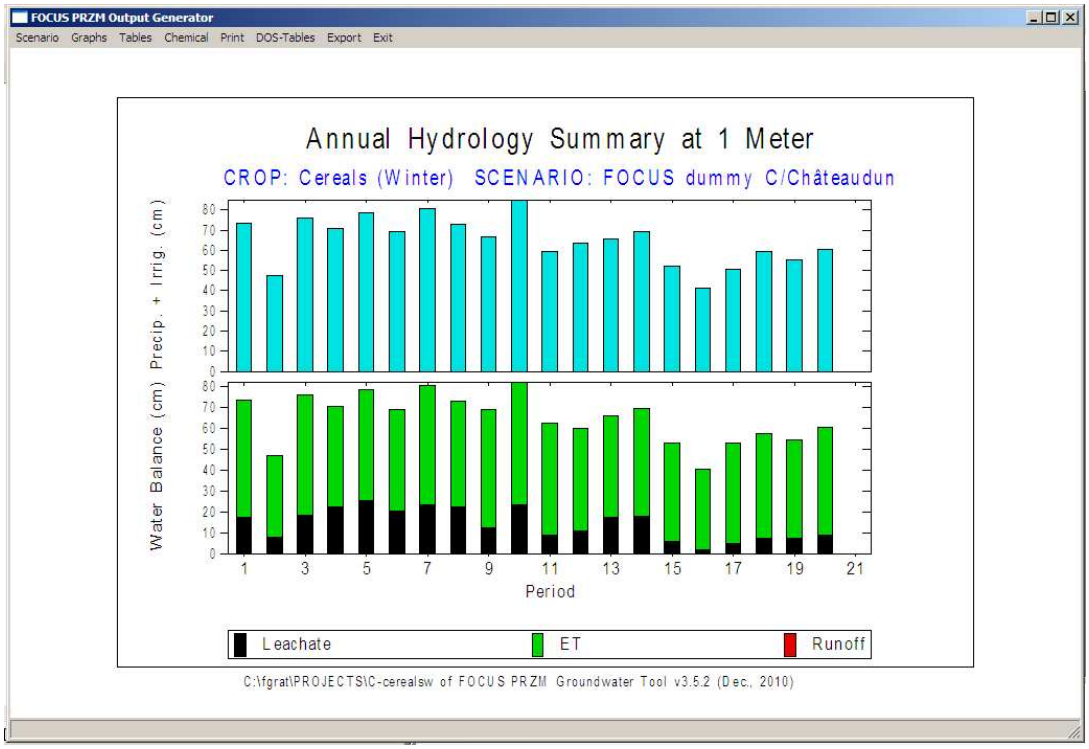
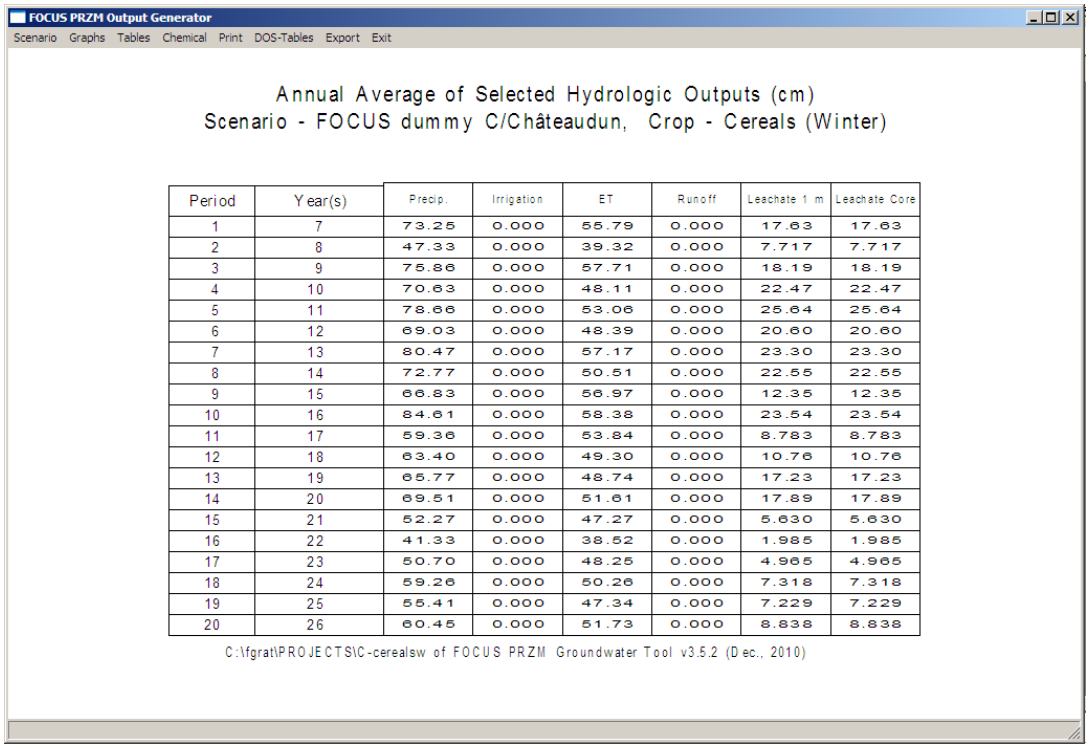


Figure 11. Graphical hydrology summary generated from the FOCUS PRZM Grapher.



Period	Year(s)	Precip.	Irrigation	ET	Runoff	Leachate 1 m	Leachate Core
1	7	73.25	0.000	55.79	0.000	17.63	17.63
2	8	47.33	0.000	39.32	0.000	7.717	7.717
3	9	75.86	0.000	57.71	0.000	18.19	18.19
4	10	70.63	0.000	48.11	0.000	22.47	22.47
5	11	78.66	0.000	53.06	0.000	25.64	25.64
6	12	69.03	0.000	48.39	0.000	20.60	20.60
7	13	80.47	0.000	57.17	0.000	23.30	23.30
8	14	72.77	0.000	50.51	0.000	22.55	22.55
9	15	66.83	0.000	56.97	0.000	12.35	12.35
10	16	84.61	0.000	58.38	0.000	23.54	23.54
11	17	59.36	0.000	53.84	0.000	8.783	8.783
12	18	63.40	0.000	49.30	0.000	10.76	10.76
13	19	65.77	0.000	48.74	0.000	17.23	17.23
14	20	69.51	0.000	51.61	0.000	17.89	17.89
15	21	52.27	0.000	47.27	0.000	5.630	5.630
16	22	41.33	0.000	38.52	0.000	1.985	1.985
17	23	50.70	0.000	48.25	0.000	4.965	4.965
18	24	59.26	0.000	50.26	0.000	7.318	7.318
19	25	55.41	0.000	47.34	0.000	7.229	7.229
20	26	60.45	0.000	51.73	0.000	8.838	8.838

Figure 12. Hydrology summary generated as a table (same data as in Figure 11).

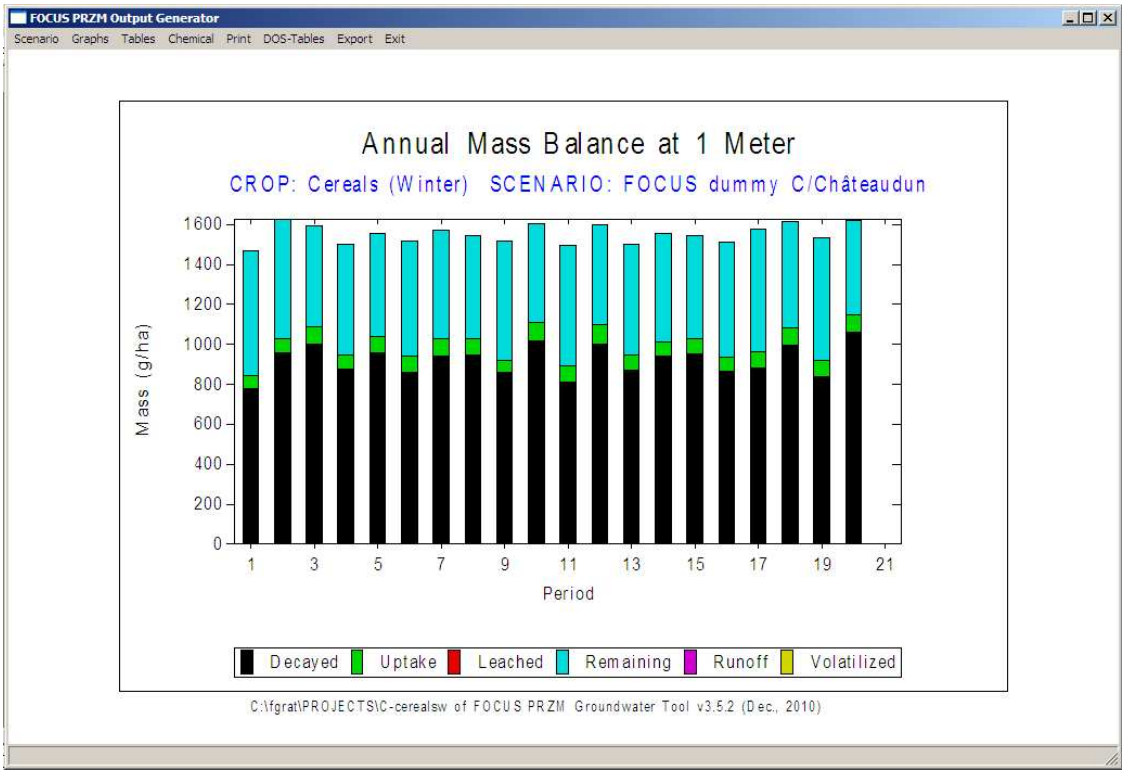
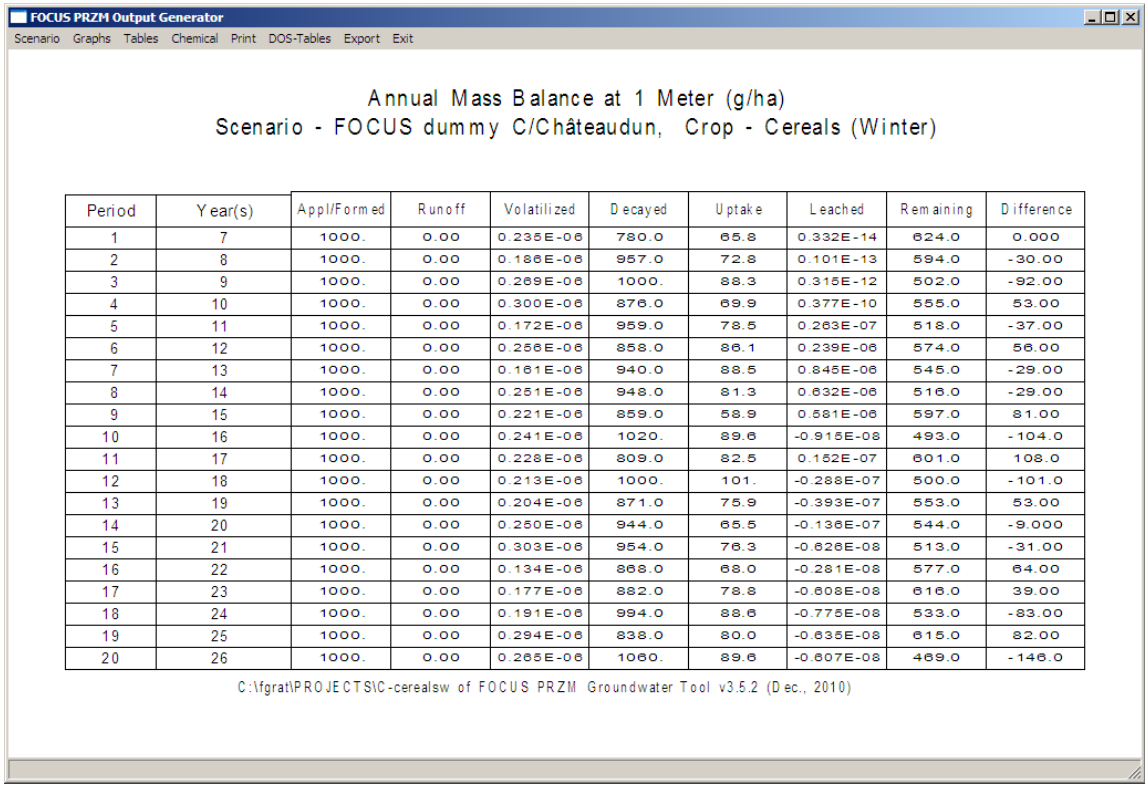


Figure 13. Graphical mass balance summary generated from the FOCUS PRZM Grapher.



Period	Year(s)	Appl/Formed	Runoff	Volatilized	Decayed	Uptake	Leached	Remaining	Difference
1	7	1000.	0.00	0.235E-06	780.0	65.8	0.332E-14	624.0	0.000
2	8	1000.	0.00	0.186E-06	957.0	72.8	0.101E-13	594.0	-30.00
3	9	1000.	0.00	0.269E-06	1000.	88.3	0.315E-12	502.0	-92.00
4	10	1000.	0.00	0.300E-06	876.0	69.9	0.377E-10	555.0	53.00
5	11	1000.	0.00	0.172E-06	959.0	78.5	0.263E-07	518.0	-37.00
6	12	1000.	0.00	0.256E-06	858.0	86.1	0.239E-06	574.0	56.00
7	13	1000.	0.00	0.161E-06	940.0	88.5	0.845E-06	545.0	-29.00
8	14	1000.	0.00	0.251E-06	948.0	81.3	0.632E-06	516.0	-29.00
9	15	1000.	0.00	0.221E-06	859.0	58.9	0.581E-06	597.0	81.00
10	16	1000.	0.00	0.241E-06	1020.	89.6	-0.915E-08	493.0	-104.0
11	17	1000.	0.00	0.228E-06	809.0	82.5	0.152E-07	601.0	108.0
12	18	1000.	0.00	0.213E-06	1000.	101.	-0.288E-07	500.0	-101.0
13	19	1000.	0.00	0.204E-06	871.0	75.9	-0.393E-07	553.0	53.00
14	20	1000.	0.00	0.250E-06	944.0	65.5	-0.136E-07	544.0	-9.000
15	21	1000.	0.00	0.303E-06	954.0	76.3	-0.626E-08	513.0	-31.00
16	22	1000.	0.00	0.134E-06	868.0	68.0	-0.281E-08	577.0	64.00
17	23	1000.	0.00	0.177E-06	882.0	78.8	-0.608E-08	616.0	39.00
18	24	1000.	0.00	0.191E-06	994.0	88.6	-0.775E-08	533.0	-83.00
19	25	1000.	0.00	0.294E-06	838.0	80.0	-0.635E-08	615.0	82.00
20	26	1000.	0.00	0.265E-06	1060.	89.6	-0.607E-08	469.0	-146.0

Figure 14. Mass balance summary generated as a table (same data as in Figure 13).

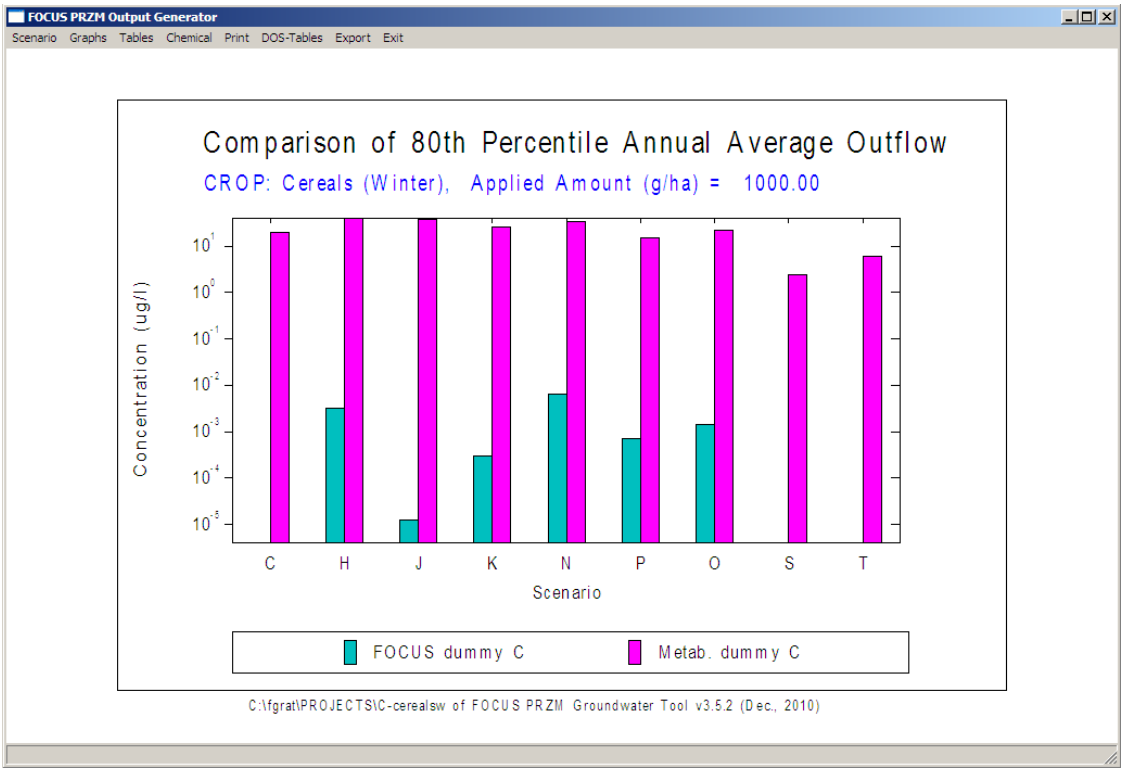


Figure 15. 80th percentile graphic generated from the FOCUS PRZM Grapher.

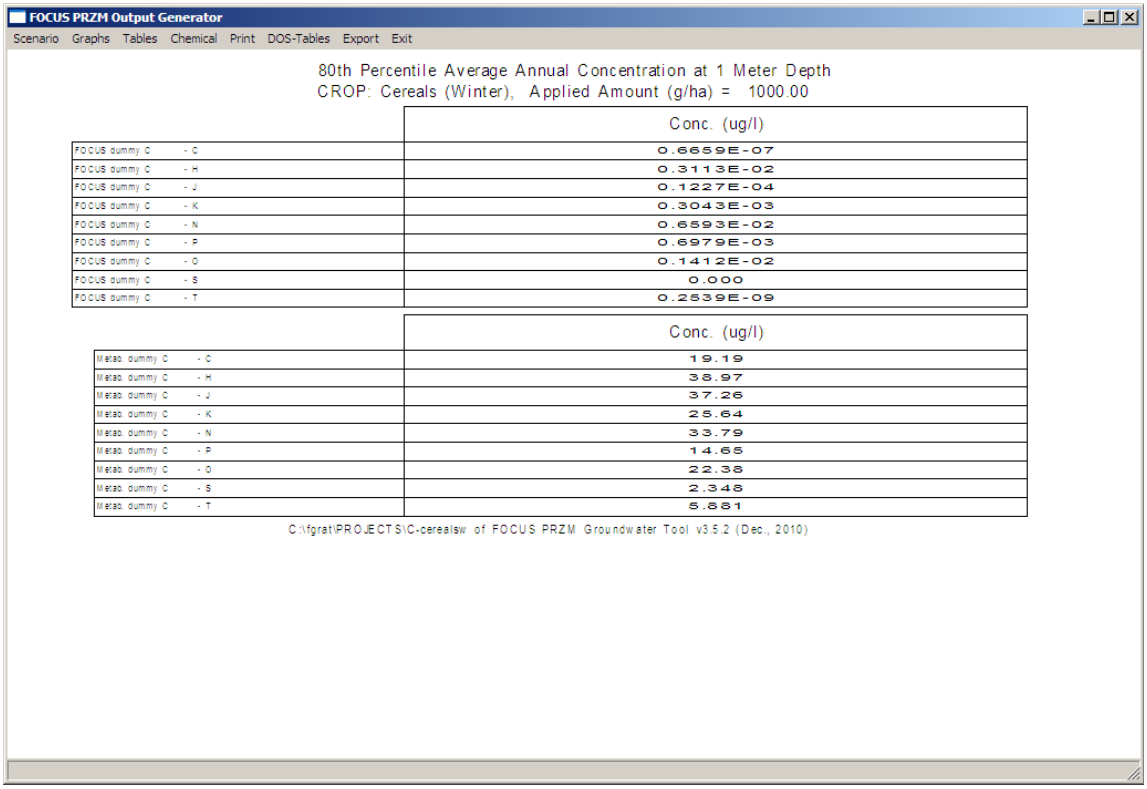


Figure 16: 80th percentile summary data generated as a table (same data as in Figure 15).