

Documentation update for PEARL 2.2.2

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1 Bugs FOCUS_PEARL_1.1.1 solved in FOCUS_PEARL_2.2.2

In FOCUS_PEARL_1.1.1 the values of the parameters HLIM3U and HLIM3L were interchanged inside the model (so a bug); in FOCUS_PEARL_2.2.2 this bug has been corrected. See the manual for the definition of these parameters.

The bug in the graph of pressure head with depth has been removed.

2 Additions and Changes to manual PEARL 1.1.1

This section describes the changes and the additions for the update of the FOCUS_PEARL_1.1.1 manual (Tiktak et al., 2000) to be used in combination with FOCUS_PEARL_2.2.2.

→ Chapter 2: Model description

In Figure 2 the name of the file 'RunId.Apo' is not correct. The name of the file is 'RunId.pfo'.

→ Section 2.3.3 Potential transpiration and potential evaporation

The extinction coefficient for global solar radiation, κ (-), has been replaced by the product of a coefficient for direct global radiation κ_{dir} (-) and a coefficient for diffuse global radiation, κ_{dif} (-). See Equations 6.25 and 6.26 in Van Dam et al. (1997).

→ Section 2.3.5 Evaporation of water from the soil surface

A second method can be used to calculate the reduction of the evaporation of water from bare soil, i.e. the method described by Black (1969):

$$\sum E_a = \beta \sqrt{t_{\text{dry}}}$$

in which:

β = empirical coefficient (cm d^{-0.5})

t_{dry} = time after significant amount of rainfall (d)

→ Section 2.5.7 Partitioning over the three soil phases

The effect of temperature on sorption coefficients can be specified via an adsorption enthalpy:

$$K_{F,e} = K_{F,e,r} \exp \left[\frac{-\Delta H_s}{R} \left(\frac{1}{T} - \frac{1}{T_r} \right) \right]$$

in which:

$K_{F,e,r}$ = the Freundlich coefficient at reference temperature T_r (K)

ΔH_s = molar enthalpy of sorption (J mol⁻¹)

In FOCUS_PEARL_2.2.2 the default value for the sorption enthalpy is zero and this gives the same calculated sorption coefficients as FOCUS_PEARL_1.1.1.

→ Chapter 3: Model parameterization

→ Section 3.2.6 Freundlich equilibrium sorption

The effect of soil temperature on the sorption coefficient can be taken into account (see above, section 2.5.7).

→ Chapter 4: User's guide for the command line version of PEARL

→ 4.2.7 Section 3: Weather and irrigation data

In FOCUS_PEARL_2.2.2 three more parameters can be specified in the input file. These parameters are:

- FacPrc: Correction factor for precipitation (-)
- DifTem: Correction for temperature (degrees Celsius)
- FacEvp: Correction factor for evapotranspiration (-)

These factors can be used to scale-up or scale-down the data on precipitation, air temperature and evapotranspiration in the file with meteorological data. The default value for FacPrc and FacEvp is set to 1.0 and the default value for DifTem is set to 0.0.

→ 4.2.8 Section 4: Boundary and initial conditions of the hydrological model

In FOCUS_PEARL_2.2.2, an additional drainage option is available, i.e. 'extended drainage'. If this option is selected then for each drainage level considered the following parameters should be specified:

- SysDra Drainage system
- RstDra Drainage resistance (d)
- RstInf Infiltration resistance (d)
- DistDra Distance between drains or channels (m)
- WidthDra Bottom width of drain system (m)
- ZDra Bottom of drain system (m)
- ZGwlInfMax Depth at which infiltration is maximal (m)
- OptSurDra Option to consider rapid subsurface drainage

If OptSurDra set to 'Yes' then the following parameters should be specified:

- RstSurDraDeep Maximum resistance of rapid subsurface drainage (d)
- RstSurDraShallow Minimum resistance of rapid subsurface drainage (d)
- OptSrfWat Option to consider surface water system

If OptSrfWat set to 'Yes' then the following parameters should be specified:

- SrfWatLevWinter Winter surface water level (m)
- SrfWatLevSummer Summer surface water level (m)
- SrfWatSupCap Surface water supply capacity (m d^{-1})

If the option 'Basic' is selected then for each drainage level considered the following additional parameters should be specified:

- RstInf Infiltration resistance (d)
- ZSurWat: Depth of the surface water table (m)

→ 4.4.3 Importing data in Excel

The selrec tool has been replaced by the sdwin tool. Using this tool, records with the same identifier can be selected and exported to an Excel file. This tool has much more possibilities, and it is also used when using the GUI. The sdwin32.exe tool is in the bin directory. Below follows a brief explanation of this tool:

sdwin32 uses a small configuration file (or setfile). This file contains lines with selection criteria as follows:

```
<datafile_name> <Column_X> <Column_Y> <Column_with_LookUpString>
<LookUpString>
```

A maximum number of 9 datapairs can be used.

For clarification the following example is given (see the format of the output files of PEARL):

```
2.out 1 4 3 Theta
```

This means that the X data are taken from column 1, the Y data are taken from column 4, and the datafile is 2.out. Only lines with Theta in the third column will be selected (Note: selection is case sensitive).

If the X-data are in the same column for all data-series, you can replace the value of Column_X with ! (except for the first data-series):

```
2.out 1 4 3 Theta
2.out ! 5 3 Theta
2.out ! 6 3 Theta
```

gives the following results (only first part of file shown)

0.000	0.2971	0.2910	0.2860
4.500	0.3039	0.3049	0.3071
11.500	0.2766	0.2824	0.2941
18.500	0.2757	0.2794	0.2885
25.500	0.2824	0.2860	0.2939
32.500	0.3399	0.3405	0.3399

sdwin32 must be called from the command line with the following arguments:

```
sdwin32 setfile -o outputfile
```

→ 4.5.1 Annual balances

The flux of each drainage system is now included in the annual water balance (see Table 10).

Table 1 Terms of the annual water balance

Field	Water balance term	Unit	Acronym
1.	Net storage change of water in the soil profile	m a^{-1}	DelLiq
2.	Precipitation flux	m a^{-1}	Prc
3.	Irrigation flux	m a^{-1}	Irr
4.	Seepage flux at the lower boundary of the system	m a^{-1}	FlvLea
5.	Evaporation flux of intercepted water	m a^{-1}	EvpInt
6.	Actual soil evaporation flux	m a^{-1}	SolAct
7.	Actual transpiration flux	m a^{-1}	TrpAct
8.	Total flux of lateral drainage to field drains and ditches	m a^{-1}	Dra
9.	Flux of lateral drainage to primary system	m a^{-1}	Dra_1
10.	Flux of lateral drainage to secondary system	m a^{-1}	Dra_2
11.	Flux of lateral drainage to tertiary system	m a^{-1}	Dra_3
12.	Flux of lateral drainage to tube drains	m a^{-1}	Dra_4
13.	Flux of lateral drainage to surface drainage system	m a^{-1}	Dra_5
14.	Flux of water in run-off	m a^{-1}	Run
15.	Evaporation of ponded water	m a^{-1}	EvpPnd
16.	Potential soil evaporation flux	m a^{-1}	SolPot
17.	Potential transpiration flux	m a^{-1}	TrpPot

Table 2 Terms of the mass balance of compounds in the soil profile. This balance applies to three different layers, i.e. the tillage layer, the FOCUS target layer and the entire soil profile. See further text.

Field	Term of mass balance ($\text{kg ha}^{-1} \text{ a}^{-1}$)	Acronym
1.	Areic mass of compound applied to the soil	AmaAppSol
2.	Areic mass change of compound in the layer	DelAma
3.	Areic mass change of compound in the equilibrium domain	DelAmaEq
4.	Areic mass change of compound in the non-equilibrium domain	DelAmaNeq
5.	Areic mass of compound transformed	AmaTra
6.	Areic mass of compound formed	AmaFor
7.	Areic mass of compound taken-up by plant roots	AmaUpt
8.	Areic mass of compound drained from the soil system	AmaDra
9.	Areic mass of compound drained from the primary system	AmaDra_1
10.	Areic mass of compound drained from the secondary system	AmaDra_2
11.	Areic mass of compound drained from the tertiary system	AmaDra_3
12.	Areic mass of compound drained from the tube drains	AmaDra_4
13.	Areic mass of compound drained from the surface drains	AmaDra_5
14.	Areic mass of compound deposited	AmaDep
15.	Areic mass of compound volatilized	AmaVol
16.	Areic mass of compound leached from the target layer	AmaLea

Hysteresis of water retention in soil can be simulated (but is switched off for FOCUS scenarios).

→ Chapter 5: User's Guide for the PEARL User Interface

→ Section 5.1: Overview of the PEARL database

The new GUI uses an Interbase database and installs Interbase on subdirectories within the tree of subdirectories of the PEARL package; thus the new GUI can work without Microsoft Access.

→ Section 5.6 The main form

The main form consists of five tabs, i.e. a scenario tab, a simulation control tab, an output control tab, a SWAP hydrological module tab and a run status tab (See Figure 1; FOCUS_PEARL_1.1.1. Manual Figure 21).

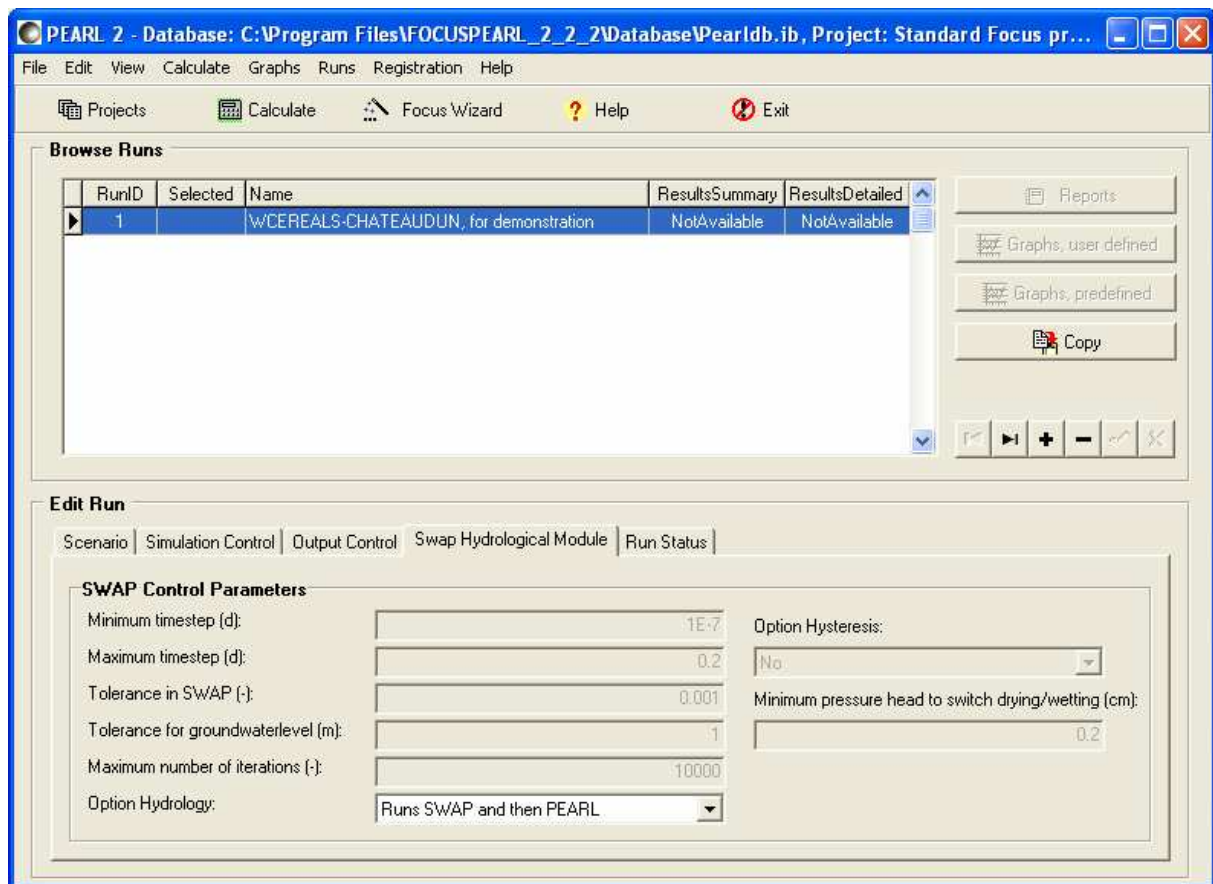


Figure 1 The main form of the PEARL user interface

On the 'SWAP hydrological module' tab, the user has to specify the option to consider hysteresis or not and the minimum pressure head to switch drying/wetting (cm). This option is switched off for FOCUS scenarios.

A facility has been added to generate an overview report of all runs in a project. After clicking on the button 'Reports', the user has to specify whether only the run selected is reported or all runs in the same project (project summary).

An archive option for runs has been added. After clicking on 'Runs' on the menu bar at the top of the main screen, the user can select 'Archive selected run'. Next the user has to specify the drive and the directory where the files should be stored.

→ **Section 5.7.1 The locations form**

A 'Copy' button has been added to copy a location.

→ **Section 5.7.1 The soil form**

The depth dependence of transformation and sorption parameters can be specified for each substance, so this dependency can be different for the parent and the metabolites (See Figure 2; FOCUS_PEARL_1.1.1. Manual Figure 23).

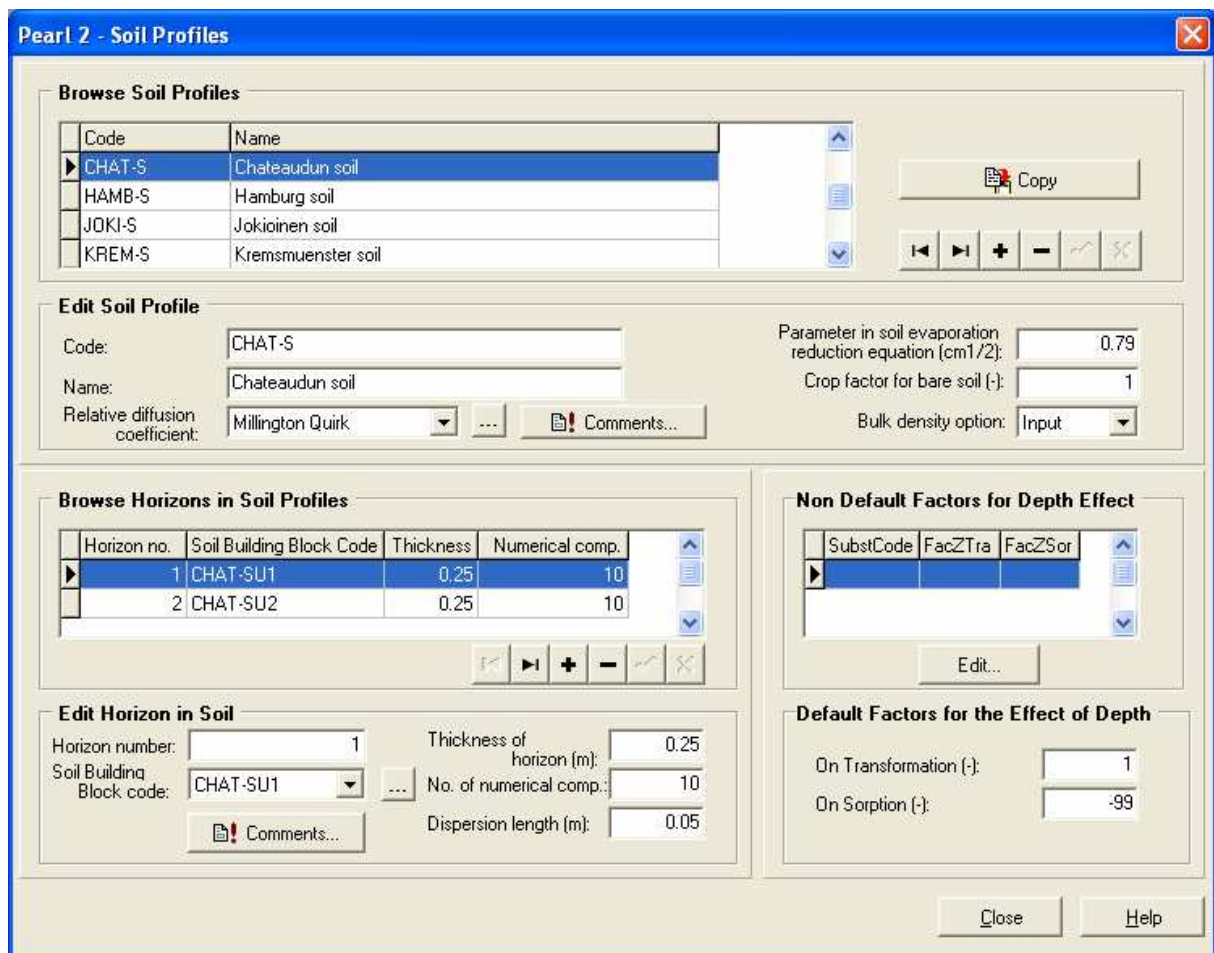


Figure 2 The Soil profiles form

→ **Section 5.8.2 The crop and development stage form**

In FOCUS_PEARL_2.2.2. the user has also to specify the depth of the virtual tensiometer and the critical pressure head for irrigation (See Figure 3; FOCUS_PEARL_1.1.1. Manual Figure 27). Both parameters are needed when using the SWAP irrigation option that calculates the irrigation amount based on prevailing soil moisture conditions.

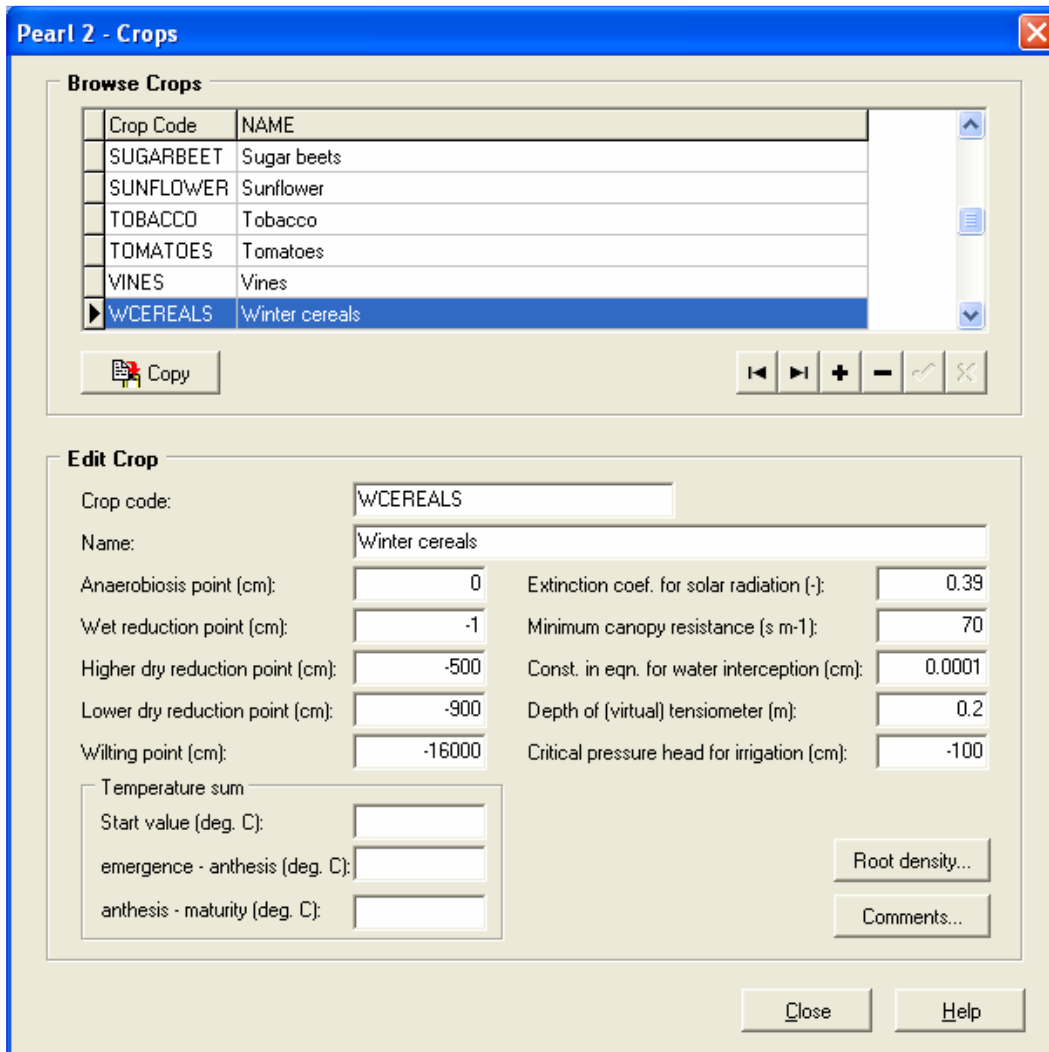


Figure 3 The crops form

→ **Section 5.9.1 Editing individual compounds**

On the 'Freundlich sorption' tab, the user has also to specify the temperature (K) at which the K_{om} value has been measured as well as the molar enthalpy of sorption (kJ mol^{-1}).

→ **Section 5.10 Editing application schemes**

The forms for editing application schemes has been graphically improved (See Figure 4; FOCUS_PEARL_1.1.1. Manual Figure 31).

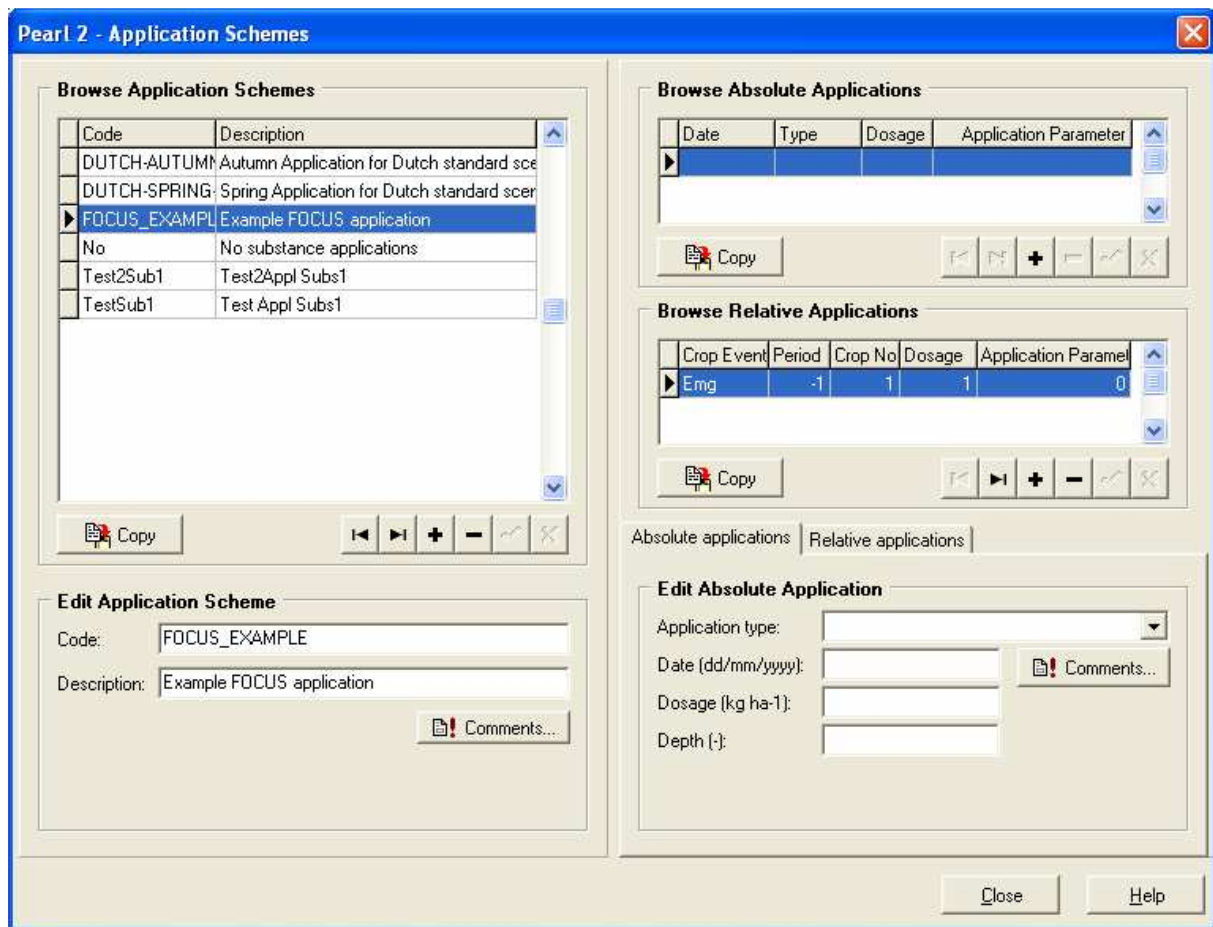


Figure 4 The application schemes form

→ **Section 5.11 Editing irrigation schemes**

On the 'Irrigation scheme' form the user can select two more options: 1) Surface irrigation, irrigation depth calculated by the model and 2) Sprinkler irrigation, irrigation depth calculated by the model. Moreover, a facility has been added to import irrigation data.

→ **Section 5.12.2 The detailed output options form**

In the category 'PEARL Concentrations' on the 'Detailed output options form', the user can now select the concentrations in the drainage water to each drain level (primary system, secondary system, etc). In the category 'PEARL Soil Balance' the areic masses drained to each drainage level can be selected for output. In the category 'SWAP Soil Fluxes' the water fluxes to each drainage level can be selected for output.

Another improvement in FOCUS_PEARL_2.2.2 is that output for all calculation nodes can be automatically generated. This facilitates making graphs of concentration and moisture profiles (See Figure 5; FOCUS_PEARL_1.1.1. Manual Figure 32).

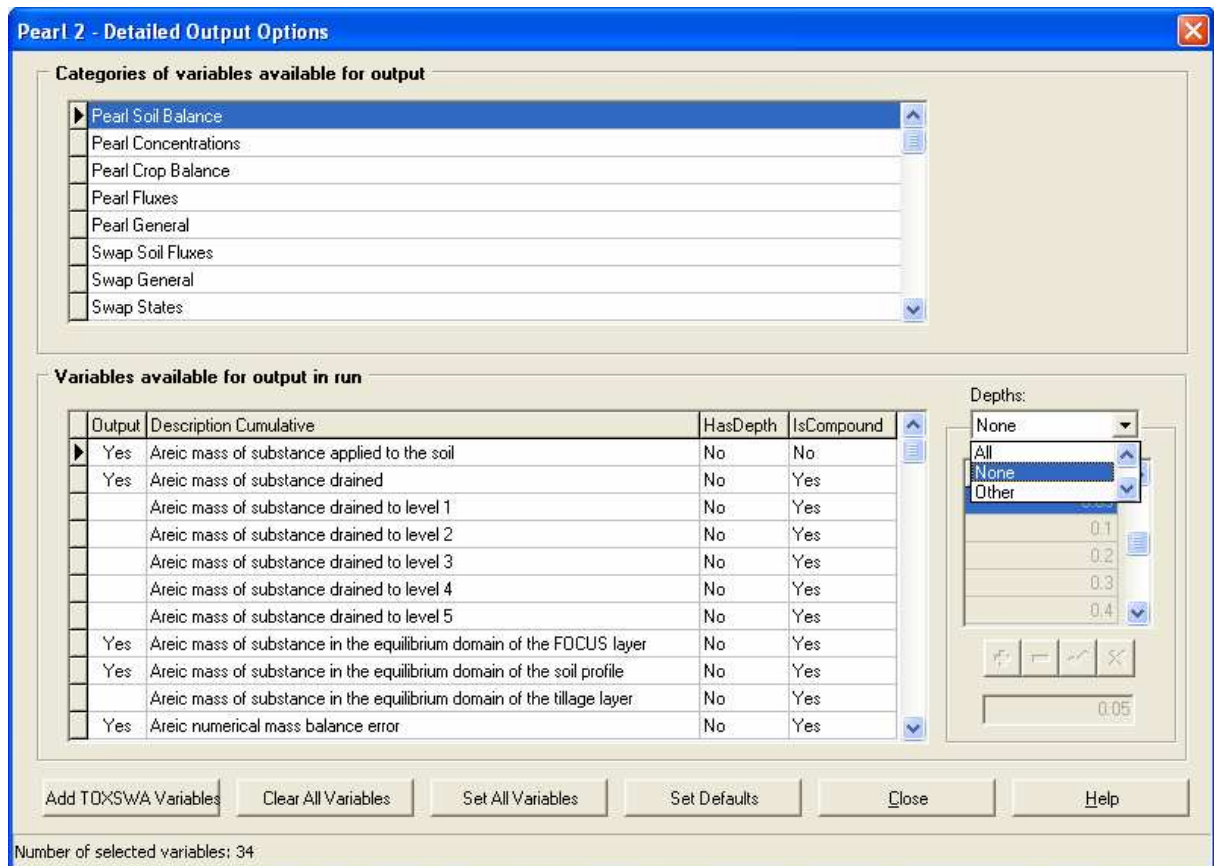


Figure 5 Output control

Literature

- Black, T.A., Gardner W.R. and Thurtell, G.W., 1969. The prediction of evaporation, drainage, and soil water storage for a bare soil. *Soil Sci. Soc. Am.*, 33, 655-660.
- Kroes, J.G., Van Dam, J.C., Huygen, J. Vervoort, R.W., 2002. User's Guide of SWAP version 2.0. Alterra-rapport 610, 137 pp. Wageningen, the Netherlands.
- Tiktak, A., Van den Berg, F., Boesten, J.J.T.I., Van Kraalingen, D., Leistra, M. & Van der Linden, A.M.A., 2000. Pesticide Emission at Regional and Local scales: Pearl version 1.1 User Manual. RIVM report 711401008, Alterra report 28.
- Dam, J.C. van, Huygen, J., Wesseling, J.G., Feddes, R.A., Kabat, P., Van Walsum, P.E.V., Groenendijk, P. & Van Diepen, C.A., 1997. SWAP version 2.0, Theory. Simulation of water flow, solute transport and plant growth in the Soil-Water-Atmosphere-Plant environment. Report 71. Department of Water Resources, Wageningen Agricultural University. Technical Document 45. DLO Winand Staring Centre, Wageningen.

3 Sensitivity analysis

FOCUS_PEARL_2.2.2 considers two conservation equations for the pesticide in the soil system, one for the equilibrium domain and one for the non-equilibrium domain (See Leistra et al. (2001) for the description of symbols):

$$\frac{\partial c_{eq}^*}{\partial t} = -R_s - \frac{\partial J_{p,L}}{\partial z} - \frac{\partial J_{p,g}}{\partial z} - R_t - R_{u,p} - R_{d,p} \quad (\text{Eq. 1})$$

$$\frac{\partial c_{ne}^*}{\partial t} = R_s \quad (\text{Eq. 2})$$

In most pesticide studies, non-equilibrium sorption is not considered, so the first term on the right-hand side of Eq. 1 can be omitted. Secondly, most of the pesticides are non-volatile, so for these compounds the transport in soil through the gas phase is much smaller than the transport through the liquid phase. Thirdly, lateral drainage is not considered in the first-tier leaching assessments at the EU-level (FOCUS groundwater scenarios), so Eq. 1 can be simplified to:

$$\frac{\partial c_{eq}^*}{\partial t} = -\frac{\partial J_{p,L}}{\partial z} - R_t - R_{u,p} \quad (\text{Eq. 3})$$

Eq. 3 is equal to the conservation equation used in the precursors of the PEARL model (PESTLA and PESTRAS) to describe the leaching of pesticide in the soil system. Therefore, a sensitivity analysis for FOCUS_PEARL_2.2.2 with the simplifications mentioned above would give the same results as a sensitivity analysis for PESTLA 1.1 and PESTRAS 3.1.

The sensitivity of calculated leaching to the parameters in the conservation equation used in PESTLA 1.1 has been assessed by Boesten (1991). His results show that the most sensitive parameters are:

- the half-life of the substance in the soil system
- the coefficient for sorption on organic matter
- the exponent in the Freundlich sorption equation

Similar sensitivity studies on pesticide behaviour in soil using Eq. 3 have been reported using the PESTRAS model by Tiktak et al. (1994) and Swartjes et al. (1993).

Literature

- Boesten, J.J.T.I., 1991. Sensitivity analysis of a mathematical model for pesticide leaching to groundwater, *Pest. Sci.* 31, 375-388.
- Leistra, M., van der Linden, A.M.A., Boesten, J.J.T.I., Tiktak, A. & Van den Berg, F. 2001. PEARL model for pesticide behaviour and emissions in soil-plant systems. Descriptions of the processes in FOCUS PEARL v 1.1.1. Alterra-Rapport 013, RIVM report 711401009.

- Tiktak, A., Swartjes, F.A., Sanders R. and Janssen, P.H.M., 1994. Sensitivity analysis of a model for pesticide leaching and accumulation. In: J. Grasman and G. van Straten (eds.). Predictability and non-linear modelling in natural sciences and economics. Kluwer Academic, Dordrecht, the Netherlands, pp. 471-484.
- Swartjes, F.A., Sanders, R., Tiktak, A. and Van der Linden, A.M.A., 1993. Modelling of leaching and accumulation of pesticides: Module selection by sensitivity analysis. In: A.A.M. Del Re, E. Capri, S.P. Evans, P. Natali, and M. Trevisan (Eds.). Proceedings IX Symposium Pesticide Chemistry: Mobility and Degradation of Xenobiotics. p. 167-181.

4 Model testing

To date, FOCUS_PEARL_2.2.2 has not been tested against measurements in field experiments. Because the concepts to describe the processes affecting the fate of the pesticide in the soil have not changed in the development from FOCUS_PEARL_1.1.1 to FOCUS_PEARL_2.2.2, the outcome of testing FOCUS_PEARL_1.1.1 as described below is valid for FOCUS_PEARL_2.2.2 too.

Bouraoui et al. (2003) have tested FOCUS_PEARL_1.1.1 to describe the behaviour of pesticides in soil using measurements from field experiments in Vredepeel (NL) and Lanna (S). In the Vredepeel field experiment, KBr, bentazon and ethoprophos were applied to a sandy soil (gley podzol) with no subsurface drainage. The model was tested using a stepwise approach (Vanclooster et al., 2003). The moisture content profiles were used to calibrate the soil hydrological parameters. Using the calibrated soil physical parameters, accurate model predictions were obtained for the bentazone and ethoprophos content profiles in the soil. For the Lanna field experiment, KBr and bentazone were applied on a silty clay soil with a drainage system. The VanGenuchten parameters n and α were calibrated using measured moisture content profiles. The dispersion length was calibrated to give a better description of the Bromide content profile. On average, the computed drain water flow was 13% less than measured. The underprediction of the drain water fluxes might be caused by the occurrence of preferential flow in the field soil, as this type of transport cannot be simulated by PEARL. The predicted concentration profile of bentazone agrees reasonably with the measurements, whereas the concentrations in the drainwater were underpredicted at times and this is probably due to the effect of preferential flow.

Scorza and Boesten (2005) have tested FOCUS_PEARL_1.1.1 against the results of a field experiment on a cracking clay soil at Andelst (NL). In this field experiment, KBr, the mobile pesticide bentazone and the moderately sorbing pesticide imidacloprid were applied to the bare soil. The model was tested using a stepwise approach (Vanclooster et al., 2003). Calibration of the soil hydrological parameters was necessary to obtain a good description of the soil moisture profiles. The dispersion length was calibrated to obtain a good description of the bromide transport in the soil. The concentrations of bentazone in the drainwater and groundwater were described reasonably well by the model. The bulk movement of imidacloprid in the soil was overestimated by the model and the concentrations of imidacloprid in drainwater was underestimated. This indicates that FOCUS_PEARL_1.1.1 cannot be used for accurate simulation of pesticide transport in cracking clay soils.

Vanclooster et al. (2003) have tested FOCUS_PEARL_1.1.1 against the results of field experiments in Bologna (I) and Brimstone (UK). In the Bologna field experiment, aclonifen and ethoprophos were applied to a loamy soil. Calibration of the soil hydrological parameters was needed to improve the description of the soil moisture profiles. The limited movement of both aclonifen and ethoprophos was reasonably described by the model. However, this experiment was not suitable to test pesticide leaching to groundwater. In the Brimstone field experiment, isoproturon was applied in different years to a cracking heavy clay soil. The soil hydrological parameters were calibrated using measured soil moisture content profiles. The average moisture content corresponded well to those measured, but at different occasions

there were large differences, presumably due to the occurrence of preferential flow. Measured concentrations of isoproturon occurred several weeks earlier than predicted by PEARL, indicating that preferential flow is an important process for this particular soil..

Literature

- Bouraoui, F., Boesten, J.J.T.I., Jarvis, N. and Bidoglio, G., 2003. Testing the PEARL model in the Netherlands and in Sweden. Proceedings XII symposium Pesticide Chemistry, Piacenza, Italy.
- Scorza Júnior, R.P. & Boesten, J.J.T.I., 2005. Simulation of pesticide leaching in a cracking clay soil with the PEARL model, *Pestic. Management Sci.*, in press.
- Vanclooster, M., Pineros-garcet, J.D., Boesten J.J.T.I., van den Berg, F., Leistra, M., Smelt, J. H., Jarvis, N., Burauel, P., Vereecken, H., Wolters, A., Linnemann, V., Fernandez, E., Trevisan, M., Capri, E., Klein, M., Tiktak, A., van der Linden A.M.A., De Nie, D., Bidoglio G., Bouraoui, F., Jones, A., Armstrong, A., 2003. Effective approaches for assessing the predicted environmental concentrations of pesticides: a proposal supporting the harmonised registration of pesticides in Europe, Final Report August 2003, 158 pp.

Appendix 1 The PEARL_2.2.2 input file – Expert users

This appendix gives a listing of the extended PEARL_2.2.2 input file. This file is intended to be used by expert users. Differences in the input file of PEARL_2.2.2 compared with PEARL_1.1.1 are set in bold face.

```

*-----
* STANDARD FILE for Pearl version 1.5.8 (16-Jun-2003).
*
* This file is intended to be used by expert users.
* Figures between brackets refer to constraints (maximum and minimum values).
*
* Pearl e-mail address: lbg-pearl@rivm.nl
*
* (c) RIVM/Alterra 7-Aug-2003
*-----

*-----
* Sector 0: Run identification
*-----

DutchRegistration      OptReport              Type of report (FOCUS, DutchRegistration)
Dutch_Location         Location                Location identification
Dutch_Soil             SoilTypeID              Soil identification
Monoculture_Maize      CropCalendar            Crop calendar
A                      SubstanceName           Substance name
One_Spring_Application ApplicationScheme        Application scheme
No                     DepositionScheme        Deposition scheme
No                     IrrigationScheme         Irrigation scheme

*-----
* Section 1: Control section
*-----

FOCUS                  CallingProgram          Release type
2                      ModelVersion           Version number of the model
2                      GUIVersion             Version number of the GUI
2                      DBVersion              Version number of the database

* Time domain
01-Jan-1980            TimStart                Begin time of simulation [01-Jan-1900|-]
31-Dec-2000            TimEnd                  End time of simulation [TimStart|-]
1.d-4                  AmaSysEnd               Stop criterion - ignored if zero [0|-]
0                      DelTimPrn               Print time step [0|-] - zero is automatic

* SWAP control
Yes                    RepeatHydrology          Repeat weather data: Yes or No
Automatic              OptHyd                  OnLine, OffLine, Stationary, Only, Automatic
1.d-5                  DelTimSwaMin            Minimum time step in SWAP [1d-8|0.1]
0.2                    DelTimSwaMax            Maximum time step in SWAP [0.01|0.5]
0.001                  ThetaTol                 Tolerance in SWAP [1e-5|0.01]
1.0                    GWLTol                  Tolerance for groundwater level
10000                  MaxItSwa                Maximum number of iterations in SWAP

Other                  OptDelTimPrn           Option to set output interval
Yes                    OptScreen              Option to write output to screen

*-----
* Section 2: Soil section
*-----

* The soil profile
* Specify for each horizon:
* Horizon thickness (m)
* The number of soil compartments [1|500]
* Nodes are distributed evenly over each horizon
table SoilProfile
ThiHor NumLay
(m)
0.3      12
0.2      8

```

0.2 4
0.3 6
2 20
end_table

* Basic soil parameters
* Specify for each soil horizon:
* Mass content of sand, expressed as a fraction of the mineral soil (kg.kg-1) [0|1]
* Mass content of silt, expressed as a fraction of the mineral soil (kg.kg-1) [0|1]
* Mass content of clay, expressed as a fraction of the mineral soil (kg.kg-1) [0|1]
* Organic matter mass content (kg.kg-1) [0|1]
* pH. pH measured in 0.01 M CaCl2 is preferred (see theory document) (-) [1|13]

table horizon SoilProperties					
Nr	FraSand (kg.kg-1)	FraSilt (kg.kg-1)	FraClay (kg.kg-1)	CntOm (kg.kg-1)	pH (-)
1	0.92	0.05	0.03	0.0470	4.7
2	0.96	0.02	0.02	0.0080	4.4
3	0.95	0.03	0.02	0.0019	4.6
4	0.94	0.04	0.02	0.0014	4.6
5	0.93	0.05	0.02	0.0000	4.6

end_table

* Parameters of the Van Genuchten-Mualem relationships (B1 + O1)
* Specify for each soil horizon:
* The saturated water content (m3.m-3) [0|0.95]
* The residual water content (m3.m-3) [0|0.04]
* Parameter alpha (cm-1) [1.d-3|1]
* Parameter n (-) [1|5]
* The saturated conductivity (m.d-1) [1.d-4|10]
* Parameter lambda (l) (-) [-25|25]
* New Starting Series - not used for standard scenario

table horizon VanGenuchtenPar							
Nr	ThetaSat (m3.m-3)	ThetaRes (m3.m-3)	AlphaDry (cm-1)	AlphaWet (cm-1)	n (-)	KSat (m.d-1)	l (-)
1	0.43	0.01	0.0249	0.0498	1.507	0.1746	-0.140
2	0.43	0.01	0.0249	0.0498	1.507	0.1746	-0.140
3	0.36	0.01	0.0224	0.0448	2.167	0.1321	0.000
4	0.36	0.01	0.0224	0.0448	2.167	0.1321	0.000

end_table

Input OptRho Calculate or Input

* If RhoOpt = Input:
table horizon Rho (kg.m-3) [100|2000]
1 1310.0
2 1540.0
3 1640.0
4 1650.0
5 1650.0
end_table

* End If

No **OptHysteresis** Option to include hysteresis
0.2 **PreHeaWetDryMin** (cm) Minimum pressure head to switch drying/wetting

* Maximum ponding depth and boundary air layer thickness (both location properties)
0.01 ZPndMax (m) Maximum ponding depth [0|1]
0.01 ThiAirBouLay (m) Boundary air layer thickness [1e-6|1]

* Soil evaporation parameters
Boesten **OptSolEvp** Option to select evaporation reduction method
1.0 FacEvpSol (-) "Crop factor" for bare soil [0.5|1.5]
0.63 CofRedEvp (cm1/2) Parameter in Boesten equation [0|1]
0.01 **PrcMinEvp** (m.d-1) Minimum rainfall to reset reduction

* Parameter values of the functions describing the relative diffusion coefficients
MillingtonQuirk OptCofDifRel MillingtonQuirk, Troeh or Currie

* If MillingtonQuirk:
2.0 ExpDifLiqMilNom (-) Exponent in nominator of equation [0.1|5]
0.67 ExpDifLiqMilDen (-) Exponent in denominator of eqn [0.1|2]
2.0 ExpDifGasMilNom (-) Exponent in nominator of equation [0.1|5]
0.67 ExpDifGasMilDen (-) Exponent in denominator of eqn [0.1|2]

* If Troeh:
0.05 CofDifLiqTro (-) Coefficient in Troeh equation [0|1]
1.4 ExpDifLiqTro (-) Exponent in Troeh equation [1|2]
0.05 CofDifGasTro (-) Coefficient in Troeh equation [0|1]

```

1.4          ExpDifGasTro      (-)          Exponent in Troeh equation      [1|2]

* If Currie:
2.5          CofDifLiqCur     (-)          Coefficient in Currie equation  [0|-]
3.0          ExpDifLiqCur     (-)          Exponent in Currie equation    [1|-]
2.5          CofDifGasCur     (-)          Coefficient in Currie equation  [0|-]
3.0          ExpDifGasCur     (-)          Exponent in Currie equation    [1|-]

* End If

* Dispersion length of solute in liquid phase [0.5Delz|1]
Table horizon LenDisLiq (m)
1  0.05
2  0.05
3  0.05
4  0.05
5  0.05
end_table

-----
* Section 3: Weather and irrigation data
-----

defscen      MeteoStation      Maximum 7 (!) characters.
Input        OptEvp             Evapotranspiration: Input, Penman or Makkink
52.0         Lat                Latitude of meteo station [-60|60]
10.0         Alt                (m)          Altitude of meteo station [-400|3000]

* Initial lower boundary soil temperature [-20|40]
* Upper boundary temperature is read from meteo file
9.97         TemLboSta         (C)

* Irrigation section
No           OptIrr
* Options for OptIrr are:
* No: no irrigation
* Surface: Surface irrigation, irrigation depth spec. by user
* Surface_Auto: Surface irrigation, irrigation depth calc. by model
* Sprinkler: Sprinkler irrigation, irrigation depth spec. by user
* Sprinkler_Auto: Sprinkler irrigation, irrigation depth calc. by model

defscen      IrrigationData      Name of file with irrigation data
* Irrigation data have to be provided in a file Station.irr (e.g. debilt.irr);
* Maximum number of characters in filename is 7.
* If RepeatHydrology is set to Yes, the first year is required only
* Format of the file should be as below:
* table IrrTab (mm)
* 01-Aug-1980 10.0
* end_table
1.0          FacPrc (-)          Correction factor for precipitation
0.0          DifTem (C)        Correction for temperature
1.0          FacEvp (-)        Correction factor for evapotranspiration
-----
* Section 4: Boundary and initial conditions of hydrological model
* Section 4a: Lower boundary flux conditions
-----

* Initial condition
1.00         ZGrwLevSta        (m)          Initial groundwater level [0|50]

* Choose one of the following options:
* GrwLev Flux Head FncGrwLev Dirichlet ZeroFlux FreeDrain Lysimeter
FncGrwLev    OptLbo           Lower boundary option

* LboOpt = GrwLev (groundwater level boundary condition)
table GrwLev (m)              Groundwater level [0|-]
01-Jan 1.00
31-Dec 1.00
end_table

* LboOpt = Flux (flux lower boundary condition)
-0.250       FlvLiqLboAvg      (m.a-1)      Average annual lower boundary flux [-1|1]
0.10         FlvLiqLboAmp      (m)          Amplitude of lower-boundary flux [0|0.5]
01-Oct       DayFlvLiqLboMax    Day of maximum flux [01-Jan|31-Dec]

* LboOpt = Head (head lower boundary condition)

```

Elliptic	OptShapeGrwLev		Elliptic, Parabolic, Sinusoidal, NoDrains
-1.1	HeaDraBase	(m)	Drainage base to correct GrwLev [-100 0]
500.0	RstAqt	(d)	Resistance of aquitard [0 1e4]
-1.4	HeaAqfAvg	(m)	Mean hydraulic head of aquifer [-10 10]
0.2	HeaAqfAmp	(m)	Amplitude of aquifer hydraulic head [0 10]
01-Apr	TimHeaAqfMax	(d)	Day with maximum head [01-Jan 31-Dec]

* LboOpt = FncGrwLev (flux boundary condition - flux is a function of groundwater level)

-0.0112	CofFncGrwLev	(m.d-1)	Coefficient in Q(h) relationship [-1 1]
-2.5	ExpFncGrwLev	(m-1)	Exponent in Q(h) relationship [-100 100]

* LboOpt = Dirichlet (pressure head boundary condition)

table	h (m)	Pressure head [-1e4 1e4]
01-Jan	-1.0	
31-Dec	-1.0	
end_table		

*-----
* Section 4b: Local drainage fluxes to ditches and drains
*-----

No	OptDra		No, Basic or extended drainage module
No	OptSurDra		Option to consider surface drainage
0	NumDraLev		Number of drainage levels (0 5)

* If OptDra set to 'Basic' parameters below should be specified for each drainage level:

1	SysDra_1		Drainage system
100.0	RstDra_1	(d)	Drainage resistance [1 1e5]
100.0	RstInf_1	(d)	Infiltration resistance
20.0	DistDra_1	(m)	Distance between drains or channels [1 1e6]
1.5	ZDra_1	(m)	Bottom of drain system [0 10]
Drain	TypDra_1		Type of drain system: Drain or Channel
1.5	ZSurWat_1	(m)	Channel water level (if TypDra_1 = Channel; otherwise dummy values)

* If OptDra set to 'Extended' parameters below should be specified for each drainage level:

1	SysDra_1		Drainage system
100.0	RstDra_1	(d)	Drainage resistance [1 1e5]
100.0	RstInf_1	(d)	Infiltration resistance
20.0	DistDra_1	(m)	Distance between drains or channels [1 1e6]
1.0	WidthDra_1	(m)	Bottom width of drain system
1.5	ZDra_1	(m)	Bottom of drain system [0 10]
1.5	ZGwlInfMax_1	(m)	Depth at which infiltration is maximal
Yes	OptSurDra		Option to consider rapid subsurface drainage

* If OptSurDra set to 'Yes' then the following parameters should be specified:

30	RstSurDraDeep	(d)	maximum resistance of rapid subsurface drainage [1e-3 1e4]]
10	RstSurDraShallow	(d)	minimum resistance of rapid subsurface drainage [1e-3 1e4]]

No	OptSrfWat		Option to consider surface water system
----	------------------	--	---

* If OptSrfWat set to 'Yes' then the following parameters should be specified:

1.0	SrfWatLevWinter	(m)	Winter surface water level
1.0	SrfWatLevSummer	(m)	Summer surface water level
0.0	SrfWatSupCap	(m.d-1)	Surface water supply capacity

*-----
* Section 5: Compound section
*-----

* Compounds. First compound is the parent pesticide, the others are metabolites.

table	compounds		
pest			
end_table			
200.0	MolMas_pest	(g.mol-1)	Molar mass [10 10000]

* Transformation table (parent-daughter relationships)
* The "end" substance is the final transformation product
* Condition: Sum of rows should be 1 (see theory document)

table	FraPrtDau (mol.mol-1)
pest	end
0.00	1.00 pest
end_table	

* Example for a pesticide with two daughters, named "met1" and "met2":
* Line 1: pest is transformed into met1 (25%), met2 (70%) and undefined end products (5%)
* Line 2: met1 is transformed into met2 (16%) and undefined end products (84%)
* Line 3: met2 is transformed into undefined end products only (100%)

```

* table FraPrtDau (mol.mol-1)
* pest met1 met2 end
* 0.00 0.25 0.70 0.05 pest
* 0.00 0.00 0.16 0.84 met1
* 0.00 0.00 0.00 1.00 met2
* end_table

* Transformation rate parameters
50.0 DT50Ref_pest (d) Half-life time [1|1e6]
20.0 TemRefTra_pest (C) Temperature at which DT50 is measured [5|30]
0.70 ExpLiqTra_pest (-) Exponent for the effect of liquid [0|5]
OptimumConditions OptCntLiqTraRef_pest OptimumConditions or NonOptimumConditions
1.0 CntLiqTraRef_pest (kg.kg-1) Liq. content at which DT50 is measured [0|1]
54.0 MolEntTra_pest (kJ.mol-1) Molar activation energy [0|200]

* Factor for the effect of depth [0|1]
table horizon FacZTra (-)
hor Pest
1 1.00
2 0.95
3 0.74
4 0.33
5 0.00
end_table

* Freundlich equilibrium sorption
pH-independent OptCofFre_pest pH-dependent, pH-independent, CofFre
1.0 ConLiqRef_pest (mg.L-1) Reference conc. in liquid phase [0.1|-]
0.9 ExpFre_pest (-) Freundlich sorption exponent [0.1|1.3]

* If pH-independent (use the coefficient for sorption on organic matter):
70.00 KomEqL_pest (L.kg-1) Coef. eql. sorption on org. matter [0|1e9]

* If pH-dependent (use pKa value and coefficient for sorption on organic matter):
374.7 KomEqLAcid_pest (L.kg-1) Coef. for eql. sorption on om - acid [0|1e9]
7.46 KomEqLBase_pest (L.kg-1) Coef. for eql. sorption on om - base [0|1e9]
4.6 pKa_pest (-) Coef. for influence of pH on sorption [0|14]
0.0 pHCorrection (-) pH correction [-2|1]

* If CofFre (specify the depth dependence and the coefficient for equilibrium sorption):
1.0 KSorEqL_pest (L.kg-1) Coef. for equilibrium sorption [0|1e9]
0.0 MolEntSor_Pest (kJ.mol-1)
20.0 TemRefsor_Pest (C)

table horizon FacZSor (-) Factor for the effect of depth [0|1]
hor Pest
1 1.00
2 0.17
3 0.04
4 0.03
5 0.00
end_table

* End If

* Gas/liquid partitioning
0.0 PreVapRef_pest (Pa) Saturated vapour pressure [0|2e5]
20.0 TemRefVap_pest (C) .. measured at [0|40]
100.0 MolEntVap_pest (kJ.mol-1) Molar enthalpy of vaporisation [-200|200]
33.0 SlbWatRef_pest (mg.L-1) Solubility in water [1e-9|1e6]
20.0 TemRefSlb_pest (C) .. measured at [0|40]
40.0 MolEntSlb_pest (kJ.mol-1) Molar enthalpy of dissolution [-200|200]

* Non-equilibrium sorption
0.00 CofDesRat_pest (d-1) Desorption rate coefficient [0|0.5]
0.5 FacSorNeqEqL_pest (-) CofFreNeq/CofFreEqL [0|-]

* Uptake
0.5 FacUpt_pest (-) Coefficient for uptake by plant [0|10]

* Canopy processes
Lumped OptDspCrp Lumped or Specified

* If Lumped:
1.d6 DT50DspCrp (d) Half-life at crop surface [1|1e6]

* If Specified:

```

```

1.d6          DT50PenCrp      (d)          Half-life due to penetration [1|1e6]
1.d6          DT50VolCrp      (d)          Half-life due to volatilization [1|1e6]
1.d6          DT50TraCrp      (d)          Half-life due to transformation [1|1e6]

* End If

1.d-4         FacWasCrp       (m-1)       Wash-off factor [1e-6|0.1]

* Diffusion of solute in liquid and gas phases
4.3d-5       CofDifWatRef_pest (m2.d-1) Reference diff. coeff. in water [10e-5|3e-4]
0.43         CofDifAirRef_pest (m2.d-1) Reference diff. coeff. in air [0.1|3]
20.0         TemRefDif_pest   (C)          Diff. coeff measured at temperature [10|30]

*-----
* Section 6: Management section
*-----
1.0          ZFoc             (m)          Depth of Focus target layer [0.1|Z(N)-1]
NoRepeat     DelTimEvt       (a)          Repeat interval of events [NoRepeat|1|2|3]

* Event table:
* If AnnualEventSameDay is set to Yes, the year is not used.

* Column 1: Date
* Column 2: Event type: AppSolSur, AppSolInj, AppSolTil, AppCrpUsr, AppCrpLAI

* If Event = AppSolSur (soil surface application):
* Column 3: Dosage (kg/ha) [0|-]

* If EventType = AppCrp (application to the crop canopy):
* Column 3: Dosage (kg/ha) [0|-]
* Column 4: Optional: Fraction of dosage applied to the crop canopy (-) [0|1]

* If EventType = AppIrr (application in irrigation water):
* Column 3: Concentration (mg/L) - checked for compatability of Irrigation table (IrrTab)

* End If

table Applications
26-May-1980 AppSolSur 1
end_table

* Tillage table - can be empty
table TillageDates
end_table

*-----
* Section 7: Initial and boundary conditions of pesticide fate model
*-----
* Initial conditions                               Concentration in equilibrium domain [0|-]

* If using metabolites, ConSysEqL should be specified for all metabolites
table interpolate CntSysEqL      (mg.kg-1)
z          pest
0.0000    0.000
5.0000    0.000
end_table

* Initial conditions                               Concentration in non-equil. domain [0|-]
* If using metabolites, ConSysNeq should be specified for all metabolites
table interpolate CntSysNeq     (mg.kg-1)
z          pest
0.0000    0.000
5.0000    0.000
end_table

* Upper boundary flux                               [0|-]
table FlmDep      (kg.ha-1.d-1)
01-Jan-1980  0.0
31-Dec-1989  0.0
end_table

* Concentration in irrigation water
0.0          ConIrr          (mg.L-1)  Concentration in irrigation water [0|-]

*-----
* Section 8: Crop section
*-----

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Yes                RepeatCrops                Repeat crop table: Yes or No

* Emergence and harvest date of crop.
* Note: Length of growing season must be constant for one crop
* If reapeat crops: Specification of year not required
table Crops
16-May-1980        04-Oct-1980    Maize
end_table

* Crop cycle fixed or variable (calculated from temperature sum)
Fixed    OptLenCrp                Fixed or Variable

* If OptLenCrp = Variable:
0.0        TemSumSta_Maize    (C)    Start value of temperature sum [-10|20]
1050.0     TemSumEmgAnt_Maize  (C)    Sum from emergence to anthesis [0|1e4]
1000.0     TemSumAntMat_Maize (C)    Sum from anthesis to maturity [0|1e4]

* End If

* Crop parameters as a function of development stage
* Column 1: Development stage: 0 = emergence; 1 = harvest (-)          [0|1]
* Column 2: LAI: Leaf Area Index (m2.m-2)                             [0|12]
* Column 3: FacCrp: Crop factor (-)                                    [0|2]
* Column 4: ZRoot: Rooting depth (m)                                  [0|10]
* Column 5: HeightCrp: Crop height (m)                               [0|10]
*      LAI  FacCrp  ZRoot  HeightCrp
table CrpPar_Maize
0.000  0.00  1.00  0.00  0.01
0.099  0.20  1.00  0.10  0.05
0.241  0.95  1.00  0.20  0.20
0.383  1.90  1.00  0.30  1.00
0.525  2.95  1.00  0.40  1.70
0.596  3.40  1.00  0.41  1.70
0.667  3.60  1.00  0.44  1.75
0.738  3.70  1.00  0.40  1.80
0.879  3.60  1.00  0.40  1.80
1.000  3.50  1.00  0.30  1.80
end_table

* Root density table (first column is relative depth)
* Column 1: Relative depth 0 = soil surface; 1 = DepRoot (-)          [0|1]
* Column 2: Root density distribution (-)                              [0|1]
Table RootDensity_Maize
0.00    1.00
1.00    1.00
end_table

* Crop water use
-10.0    HLim1_Maize    (cm)    Anaerobiosis point [-100|0]
25.0     HLim2_Maize    (cm)    Wet reduction point [-1000|0]
-1000.0  HLim3L_Maize   (cm)    Dry reduction point [-10000|0]
-1000.0  HLim3U_Maize   (cm)    Dry reduction point [-10000|0]
-8000.0  HLim4_Maize    (cm)    Wilting point [-16000|0]

70.0     RstEvpCrp_Maize (s.m-1)    Min. canopy resistance [0|1000]
0.5325   CofExtDif_Maize (-)
1.0      CofExtDir_Maize (-)
0.2      ZTensioMeter_Maize (m)
100.0    PreHeaIrrSta_Maize (cm)
1.d-4    CofIntCrp_Maize                Constant in Braden eq for interception [0|1]

-----
* Section 9: Output control
-----

* First, specify the time format in the output file:
* DaysFromSta : Print number of days since start of simulation
* DaysFrom1900 : Print number of days since 1900
* Years       : Print years
DaysFromSta   DateFormat                Format of time column in output file
No            OptDelOutput
Yes          PrintCumulatives

table VerticalProfiles
end_table

```

```

* Format of the ordinary output - use FORTRAN notation:
* e is scientific notation, g = general is general notation
* Then follow the number of positions
* Then the number of digits
g12.4          RealFormat          Format of ordinary output

* Second, specify the nodal heights for which output is requested
table OutputDepths (m)
0.05
0.10
0.15
0.20
0.25
0.50
1.00
1.50
2.00
3.00
end_table

* Finally, specify for all variables whether output is wanted (Yes or No)
* As Pearl can potentially generate large output files, it is recommended to minimise
* the number of output variables

* Section I : Output from the SWAP model, version 2.0.7c

* General variables
No          print_GrwLev          Groundwater level (m)
No          print_LAI             Leaf Area Index (m2.m-2)
No          print_ZRoot           Rooting depth (m)
No          print_FacCrpEvp        Crop factor (-)
No          print_FraCovCrp        Soil cover (-)
No          print_AvoLiqErr        Water balance error (m)
No          print_StoCap          Phreatic storage capacity (m3.m-2)
* State variables
No          print_Tem              Soil temperature (C)
No          print_Eps              Volumic air content (m3.m-3)
No          print_Theta            Volumic soil water content (m3.m-3)
No          print_PreHea           Soil water pressure head (m)

* Volumic volume rates (m3.m-3.d-1)
Yes         print_VvrLiqDra        Volumic volume rate of drainage
Yes         print_VvrLiqUpt        Volume flux of water uptake

* Volume fluxes (m3.m-2.d-1)
No          print_FlvLiq           Volume flux of vertical soil water flow
No          print_FlvLiqPrc        Volume flux of precipitation
No          print_FlvLiqIrr        Volume flux of water in irrigation
No          print_FlvLiqLbo        Volume flux of water leaching from the soil system
No          print_FlvLiqEvpIntPrc  Evaporation flux of intercepted rainfall
No          print_FlvLiqEvpIntIrr  Evaporation flux of intercepted irrigation
No          print_FlvLiqEvpSol     Volume flux of evaporation from the soil surface
No          print_FlvLiqEvpSolPot  Idem, potential
No          print_FlvLiqTrp        Volume flux of transpiration by plant roots
No          print_FlvLiqTrpPot     Idem, potential
No          print_FlvLiqDra_1      Volume flux of drainage to level 1
No          print_FlvLiqDra_2      Volume flux of drainage to level 2
No          print_FlvLiqDra_3      Volume flux of drainage to level 3
No          print_FlvLiqDra_4      Volume flux of drainage to level 4
No          print_FlvLiqDra_5      Volume flux of drainage to level 5
No          print_FlvLiqGrw      Volume flux groundwater recharge

* Section II : Output from the PEARL model
* Remark: All fluxes are averages over the print interval
*-----

* Time step
No          print_DelTimPrl        Average time-step during the print interval (d)

* Mass balance (kg.m-2)
Yes         print_AmaEqLPro        Areic mass in equilibrium domain of profile
Yes         print_AmaEqLTil        Areic mass in equilibrium domain of tillage layer
Yes         print_AmaEqLFoc        Areic mass in equilibrium domain of focus layer
Yes         print_AmaNeqPro        Areic mass in non-eql. domain of profile
Yes         print_AmaNeqTil        Areic mass in non-eql. domain of tillage layer
Yes         print_AmaNeqFoc        Areic mass in non-eql. domain of focus layer
Yes         print_AmaSysPro        Areic mass of pesticide in the system

```

Yes	print_AmaSysTil	Areic mass of pesticide in the tillage layer
Yes	print_AmaSysFoc	Areic mass of pesticide in the focus layer
Yes	print_AmaAppSol	Areic mass applied to the soil system
Yes	print_AmaDraPro	Areic mass of lateral discharge
Yes	print_AmaForPro	Areic mass of formation
Yes	print_AmaTraPro	Areic mass of pesticide transformation
Yes	print_AmaUptPro	Areic mass of pesticide uptake
Yes	print_AmaDra_1	Areic mass of drainage to level 1
Yes	print_AmaDra_2	Areic mass of drainage to level 2
Yes	print_AmaDra_3	Areic mass of drainage to level 3
Yes	print_AmaDra_4	Areic mass of drainage to level 4
Yes	print_AmaDra_5	Areic mass of drainage to level 5
Yes	print_AmaErrPro	Areic numerical mass error
* Pesticide concentrations (kg.m-3) and contents (kg.kg-1)		
No	print_ConLiq	Concentration in liquid phase
No	print_ConGas	Concentration in gas phase
No	print_ConSysEqL	Concentration in equilibrium domain
No	print_ConSysNeq	Concentration in non-equilibrium domain
No	print_ConSys	Concentration in the soil system
No	print_CntSorEqL	Mass content at soil solid phase
No	print_ConLiqSatAvg	Avg. conc.in liq. phase between 1-2 m
* Pesticide mass fluxes (kg.m-2.d-1)		
No	print_FlmLiq	Pesticide mass flux in liquid phase
No	print_FlmGas	Pesticide mass flux in gas phase
No	print_FlmSys	Total pesticide mass flux (FlmLiq+FlmGas)
No	print_FlmLiqLbo	Accumulated mass flux at the lower boundary
No	print_FlmLiqInf	Accumulated mass flux of pesticide infiltration
No	print_FlmGasVol	Accumulated mass flux of pesticide volatilisation
* Canopy interaction		
*-----		
No	print_AmaCrp	Areic mass of pesticide at the canopy
No	print_AmaAppCrp	Areic mass of pesticide applied to the canopy
No	print_AmrDspCrp	Areic mass rate of pesticide dissipation
No	print_AmaHarCrp	Areic mass rate of pesticide removal by harvest
No	print_AmrWasCrp	Areic mass rate of pesticide wash-off
No	print_FlmDepCrp	Areic mass rate of pesticide deposited on canopy
*-----		
* End of Pearl input file		
*-----		