Documentation update for PEARL 3.3.3

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1 Bugs FOCUS_PEARL_2.2.2 solved in FOCUS_PEARL_3.3.3

In FOCUS_PEARL_2.2.2 occasionally a run failure occurred for substances (parents or metabolites) with Freundlich exponents exceeding 1.0. The subroutine for the calculation of the time step in PEARL has been improved, so this error will no longer occur. Furthermore, the calculation of the temperature-dependency of the sorption coefficient contained an error. Whether the molar enthalpy of sorption was set to zero or not, all calculations were performed with a sorption coefficient that was no function of temperature. This error has been eliminated, so the temperature-dependency of the sorption coefficient is now taken into account.

2 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.

3 Additions and Changes to manual FOCUS_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_3.3.3.

3.1 \rightarrow 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'.

3.1.1 \rightarrow 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Potential transpiration and potential evaporation The extinction coefficient for global solar radiation, κ (-), has been replaced by the product of a coefficient for direct global radiation κ_{dir} (-) and a coefficient for diffuse global radiation, κ_{dif} (-).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).

3.1.2 \rightarrow 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):

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

in which:

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

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

3.1.3 \rightarrow 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_3.3.3 the default value for the sorption enthalpy is zero and this gives the same calculated sorption coefficients as FOCUS_PEARL_1.1.1.

3.2 \rightarrow Chapter 3: Model parameterization

3.2.1 \rightarrow Section 3.2.6 Freundlich equilibrium sorption

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

$3.3 \rightarrow$ Chapter 4: User's guide for the command line version of PEARL

3.3.1 \rightarrow 4.2.4 Section 1: Simulation control

In FOCUS_PEARL_3.3.3, an additional parameter is available to specify the number of years in the warming-up period. Two parameters that are used in SWAP: specification of the number of iterations and the tolerance in the procedure to calculate the groundwater level. The parameter 'AcceptDefaults' has been removed.

3.3.2 \rightarrow 4.2.6 Section 2: Soil properties and soil profile

In FOCUS_PEARL_3.3.3, the user has the possibility to consider hysteresis in the description of the water retention curve. Therefore, in the table with the Van Genuchten parameters, a column has been added with values for the parameter alpha of the wetting part of the curve , i.e. AlphaWet. The parameter Alpha in this table has been renamed to AlphaDry. When considering hysteresis, the user has also to specify the minimum pressure head to switch from the drying to the wetting part of the curve.

3.3.3 \rightarrow **4.2.7** Section 3: Weather and irrigation data

In FOCUS_PEARL_3.3.3 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.

3.3.4 → 4.2.8 Section 4: Boundary and initial conditions of the hydrological model

In FOCUS_PEARL_3.3.3, 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)

3.3.5 → **4.2.9** Section **5**: Compound properties

In FOCUS_PEARL_3.3.3, an additional option is available to set the value for the half-life of the compound in the soil. The value for the half-life can be specified in the pearl input file, or it can be set to depend on organic matter content, clay content and pH (Tiktak et al., 2003). This option is not available in the GUI of FOCUS_PEARL_3.3.3.

Two more parameters have been added to describe the temperature dependency of the sorption coefficient, namely the molar enthalpy of sorption and the temperature at which the sorption coefficient was obtained.

3.3.6 \rightarrow **4.2.13** Section 9: Control of daily output

In FOCUS_PEARL_3.3.3, the amount of water in the soil and the phreatic storage capacity can be written to the output file.

3.3.7 \rightarrow 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

3.3.8 \rightarrow **4.5.1** Annual balances

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

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 tertairy 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 1 Terms of the annual water balance

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 (kg ha ⁻¹ 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	DelAmaEql
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 volatized	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).

3.4 \rightarrow Chapter 5: User's Guide for the PEARL User Interface

3.4.1 \rightarrow 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.

3.4.2 \rightarrow 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).

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owse Runs				
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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.

3.4.3 \rightarrow Section 5.7.1 The locations form

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

3.4.4 \rightarrow 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).

	Name	~
CHAT-S	Chateaudun soil	Сору
HAMB-S	Hamburg soil	
JOKI-S	Jokioinen soil	
KREM-S	Kremsmuenster soil	
Edit Soil Profi	e	
Code:	CHAT-S	Parameter in soil evaporation reduction equation (cm1/2): 0.79
Name:	Chateaudun soil	Crop factor for bare soil (-):
Relative diffusio		Bulk density option: Input
	ons in Soil Profiles	Non Default Factors for Depth Effect
Horizon no.	Soil Building Block Code Thickness Numerical comp. CHAT-SU1 CHAT-SU2 CHAT-	SubstCode FacZTra FacZSor
Horizon no.	Soil Building Block Code Thickness Numerical comp.	SubstCode FacZTra FacZSor
Horizon no.	Soil Building Block Code Thickness Numerical comp. CHAT-SU1 0.25 10 CHAT-SU2 0.25 10 CHAT-SU2 0.25 X0 V	SubstCode FacZTra FacZSor
Horizon no. 1 2 Edit Horizon in Iorizon number:	Soil Building Block Code Thickness Numerical comp. CHAT-SU1 0.25 10 CHAT-SU2 0.25 10 CHAT-SU2 0.25 X Soil	SubstCode FacZTra FacZSor
Horizon no.	Soil Building Block Code Thickness Numerical comp. CHAT-SU1 0.25 10 CHAT-SU2 0.25 10 CHAT-SU2 0.25 10 Soil	SubstCode FacZTra FacZSor

Figure 2 The Soil profiles form

3.4.5 \rightarrow Section 5.8.2 The crop and development stage form

In FOCUS_PEARL_3.3.3. 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.

PEARL 3 - Crops	RL 3 - Crops						
Browse Crops					-		
Crop Code	NAME						
SUGARBEET	Sugar beets						
SUNFLOWER	Sunflower						
TOBACCO	Tobacco						
TOMATOES	Tomatoes						
VINES	Vines						
► WCEREALS	Winter cereal	s		~			
📑 Сору							
Edit Crop					7		
Crop code:		WCEREALS					
Name:		Winter cereals					
Anaerobiosis point	: (cm):	0	Extinction coef. for solar radiation (-):	0.39			
Wet reduction poir	nt (cm):	-1	Minimum canopy resistance (s m-1):	70			
Higher dry reduction	on point (cm):	-500	Const. in eqn. for water interception (cm):	0.0001			
Lower dry reductio	on point (cm):	-900	Depth of (virtual) tensiometer (m):	0.2			
Wilting point (cm):		-16000	Critical pressure head for irrigation (cm):	-100			
Temperature sur	m						
Start value (deg.	. C):						
emergence - ant	thesis (deg. C):		R	oot density			
anthesis - maturi	ity (deg. C):			Comments			
			<u>C</u> lose	Help			

Figure 3 The crops form

3.4.6 → Section **5.9.1** Editing individual compounds

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

3.4.7 → 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).

Teachers and	1		1	-	č.	100		
Code	Description		<u>^</u>		Date	Туре	Dosage	Application Parameter
	UTUMN Autumn Application for		4					_ _
	PRING Spring Application for XAMPLExample FOCUS appli							
No	No substance applicat	and the second se		1¢	Eba -	. F		
100		Jon 5	-	-	📴 Сору			
				Br	owse Re	lative App	olications	
				-	Crop Eve	nt Period I	Crop No Dosa	age Application Paramel
					Emg			1 Application Paramet
				ľ	Ling	N MIR	()Wit	- 104
								8
			177781		📴 Сору			K H + - 28
				-	-4-1 FJ			
📴 Сору	H	H + - ~	8	Absol	ute applica	itions Rela	ative applicati	ons
		at at at a				1		
dit Applica	ation Scheme			E	lit Absolu	te Applic	ation	
ode:	FOCUS EXAMPLE		_	Ap	plication ty	/pe:		
			_	Da	ite (dd/mm	1/9999):		B! Comments
escription:	Example FOCUS application			De	osage (kg ł	na-1):		
		📑 Commen	its			-		
				De	pth (-):			

Figure 4 The application schemes form

3.4.8 → 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.

3.4.9 \rightarrow 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_3.3.3 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).

and sourcess	Soil Balance			^	
	Concentrations				
-	Crop Balance			1	
Pearl					
1.1.1.1.1.1.1	General				
	Soil Fluxes			1	
-	General			1	
Swap	States			~	
Outpu • Yes	available for output in run t Description Cumulative Areic mass of substance applied to the soil	HasDepth No	No		Depths:
Outpu	t Description Cumulative Areic mass of substance applied to the soil Areic mass of substance drained Areic mass of substance drained to level 1	No No No	No Yes Yes		Other
Outpu Yes	t Description Cumulative Areic mass of substance applied to the soil Areic mass of substance drained Areic mass of substance drained to level 1 Areic mass of substance drained to level 2	No No No No	No Yes Yes Yes		Other All Other
Outpu Yes	t Description Cumulative Areic mass of substance applied to the soil Areic mass of substance drained Areic mass of substance drained to level 1	No No No	No Yes Yes		Other All All None Other 0.1
Outpu Yes	t Description Cumulative Areic mass of substance applied to the soil Areic mass of substance drained Areic mass of substance drained to level 1 Areic mass of substance drained to level 2 Areic mass of substance drained to level 3	No No No No No	No Yes Yes Yes Yes		Other Cher
Outpu Yes Yes	t Description Cumulative Areic mass of substance applied to the soil Areic mass of substance drained Areic mass of substance drained to level 1 Areic mass of substance drained to level 2 Areic mass of substance drained to level 3 Areic mass of substance drained to level 4	No No No No No No	No Yes Yes Yes Yes Yes		Other All None Other 0.1 0.2 0.3
Outpu Yes Yes	t Description Cumulative Areic mass of substance applied to the soil Areic mass of substance drained Areic mass of substance drained to level 1 Areic mass of substance drained to level 2 Areic mass of substance drained to level 3 Areic mass of substance drained to level 4 Areic mass of substance drained to level 5 Areic mass of substance in the equilibrium domain of the FOCUS layer	No No No No No No No	No Yes Yes Yes Yes Yes Yes		Other All None Other 0.1 0.2 0.3
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Figure 5 Output control

3.5 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.
- Dam, J.C. Van, Huygen, J., Wesseling, J.G., Feddes, R.A., Kabat, P., Van Walsum, P.E.V., Groenendijk, P. and 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.
- Kroes, J.G., Van Dam, J.C., Huygen, J. and R.W. Vervoort, 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. and 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.
- Tiktak, A., Van der Linden, A.M.A. and Boesten, J.J.T.I., 2003. The GeoPEARL model. Model description, applications and manual

4 Sensitivity analysis

FOCUS_PEARL_3.3.3 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):

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

$$\frac{\partial c_{eq}^*}{\partial t} = -\frac{\partial J_{p,L}}{\partial z} - R_t - R_{u,p}$$
(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_3.3.3 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).

4.1 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.

5 Model testing

To date, FOCUS_PEARL_3.3.3 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_3.3.3, the outcome of testing FOCUS_PEARL_1.1.1 as described below is valid for FOCUS_PEARL_3.3.3 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.

5.1 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.

6 Appendix 1 The PEARL_3.3.3 input file – Expert users

This appendix gives a listing of the extended PEARL_3.3.3 input file. This file is intended to be used by expert users. Differences in the input file of PEARL_3.3.3 compared with PEARL_1.1.1 are set in bold face.

```
_____
* Input file for Pearl 3.3.3
* This file is intended to be used by expert users.
* Figures between brackets refer to constraints (maximum and minimum values).
* Pearl e-mail address: pearl@pesticidemodels.nl
* (c) RIVM/MNP/Alterra April-2006
*_____
* Goto section:
 Section 0: Run identification and FOCUS version
* Section 1: Control section
* Section 2: Soil section
* Section 3: Weather and irrigation data
* Section 4: Boundary and initial conditions of hydrological model
 Section 5: Compound section
* Section 6: Management section
* Section 7: Initial and boundary conditions of pesticide fate model
* Section 8: Crop section
* Section 9: Output control
*_____
* Section 0: Run identification
*_____
                        _____
FOCUS
                                    Type of report (No, FOCUS, DutchRegistration)
                   OptReport
HAMBURG
                   Location
                                    Location identification
                   SoilTypeID
                                    Soil identification
HAMB-S Soil
                                   Crop calendar
HAMB-WCEREALS
                  CropCalendar
pest
                  SubstanceName
                                   Substance name
FOCUS_EXAMPLE
                  ApplicationScheme Application scheme
No
                  DepositionScheme Deposition scheme
NΟ
                   IrrigationScheme
                                    Irrigation scheme
*_____
* Section 1: Control section
* Description
*_____
FOCUS
              CallingProgram
                                    Release type
                                     Version number of the model
              ModelVersion
3
                                     Version number of the GUI
3
              GUIVersion
3
              DBVersion
                                     Version number of the database
* Time domain
             TimStart
                                    Begin time of simulation [01-Jan-1900 -]
01-Jan-1901
31-Dec-1926
             TimEnd
                                     End time of simulation [TimStart | - ]
              InitYears
                                     Number of years in warming-up period
б
                                    Stop criterion - ignored if zero [0]-]
1.d-4
              AmaSysEnd
                       (kg.ha-1)
              DelTimPrn
                                    Print time step [0]-] - zero is automatic
1
                        (d)
* SWAP control
No
              RepeatHydrology
                                    Repeat weather data: Yes or No
Automatic
              0pt.Hvd
                                    OnLine, OffLine, Stationary, Only, Automatic
              DelTimSwaMin (d)
                                    Minimum time step in SWAP [1d-8|0.1]
1.d-5
0.2
              DelTimSwaMax (d)
                                    Maximum time step in SWAP [0.01 0.5]
0.001
             ThetaTol (m3.m-3)
                                    Tolerance in SWAP [1e-5|0.01]
              GWLTol
                                     Tolerance for groundwater level
1.0
                        (m)
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
* Description
* 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)
         12
0.3
0.1
         4
0.2
          8
0.2
          4
          4
0.2
        35
3.5
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]
                                                                             (kg.kg-1) [0|1]
* Organic matter mass content
^{\ast} pH. pH measured in 0.01 M CaCl2 is preferred (see theory document) (-)
                                                                                         [1]13]
table horizon SoilProperties
       FraSand FraSilt FraClay
Nr
                                          CntOm
                                                            pН

      Frasand
      Frasht
      Frasht
      Frasht
      Frasht
      Encom

      (kg.kg-1)
      (kg.kg-1)
      (kg.kg-1)
      (kg.kg-1)
      (kg.kg-1)

      0.683
      0.245
      0.072
      0.026

      0.67
      0.263
      0.067
      0.017

      0.962
      0.029
      0.009
      0.0034

      0.998
      0.002
      0
      0

                                                            (-)
1
                                                            -99
2
      0.67
                                                            -99
3
                                                            -99
      0.998
4
                                                            -99
       1
                                0
5
                   0
                                            0
                                                            -99
б
       1
                    0
                                0
                                            0
                                                            -99
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 AlphaDry
                                     (cm-1) [1.d-3|1]
* Parameter AlphaWet
                                     (cm-1)
                                                [1.d-3|1]
* Parameter n
                                     ( – )
                                                [1|5]
                                   (m.d-1)
(-)
                                                [1.d-4|10]
[-25|25]
* The saturated conductivity
* Parameter lambda (l)
* New Staring Series - not used for standard scenario
table horizon VanGenuchtenPar
                                                       . KSat
(-) '
Nr ThetaSat ThetaRes AlphaDry AlphaWet n
                                                                            1
                                                                (m.d-1)
   (m3.m-3)
               (m3.m-3)
                                         (cm-1)
                                                                            ( – )
                            (cm-1)
                                                       (, (m.u-1) (-)

1.468 2.016 0.5

1.565 2.736 0.5

1.598 2.448 0.5
                             0.0149 0.0298
1
      0.391
                   0.036
2
       0.37
                     0.03
                                  0.0126
                                              0.0252
                                              0.0362
3
       0.351
                    0.029
                                 0.0181
                                                         1.606
4
       0.31
                    0.015
                                  0.0281
                                              0.0562
                                                                    2.448
                                                                              0.5
                    0.015
                                              0.0562
5
       0.31
                                  0.0281
                                                           1.606
                                                                    2.448
                                                                              0.5
б
       0.31
                    0.015
                                  0.0281
                                             0.0562
                                                           1.606
                                                                    2.448
                                                                              0.5
end_table
                   Opt.Rho
                                                   Calculate or Input
Input
* If RhoOpt = Input:
                                    (kg.m-3) [100|2000]
table horizon
                   Rho
1 1500.0
2
     1600.0
     1560.0
3
4
     1620.0
5
     1600.0
6
    1600.0
end_table
* End If
                    OptHysteresis
                                                   Option to include hysteresis
No
0.2
                   PreHeaWetDryMin (cm)
                                                  Minimum pressure head to switch drying/wetting
```

```
* Maximum ponding depth and boundary air layer thickness (both location properties)
0.002
                 ZPndMax
                                           Maximum ponding depth [0|1]
                                (m)
0.01
                 ThiAirBouLav
                                 (m)
                                            Boundary air layer thickness [1e-6|1]
* Soil evaporation parameters
Boesten
                 OptSolEvp
                                             Option to select evaporation reduction method
                                             "Crop factor" for bare soil [0.5|1.5]
                                 ( - )
1.0
                 FacEvpSol
                 CofRedEvp
0.79
                                 (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
                 ExpDifLigMilDen (-)
                                            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]
                               ( - )
                                            Exponent in Troeh equation
1.4
                 ExpDifGasTro
                                                                             [1|2]
* If Currie:
2.5
                 CofDifLiqCur (-)
                                            Coefficient in Currie equation [0]-]
3.0
                 ExpDifLiqCur (-)
                                            Exponent in Currie equation
                                                                             [1|-]
                 CofDifGasCur (-)
2.5
                                            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
6 0.05
end_table
*_____
* Section 3: Weather and irrigation data
* Description
*_____
HAMB-M
                 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
5.3
                 TemLboSta
                                (C)
* Irrigation section
                 OptIrr
No
* 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
                                        Correction for temperature
                DifTem (C)
1.0
                FacEvp (-)
                                         Correction factor for evapotranspiration
*____
                                     _____
* Section 4: Boundary and initial conditions of hydrological model
* Section 4a: Lower boundary flux conditions
* Description
                      _____
* Initial condition
-200
                ZGrwLevSta
                             (cm)
                                       Initial groundwater level [-5000 0]
* 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)
* Read from LowerBoundaryFile (RunId.bot)
[Run Td]
* table
        GrwLev
                 ( cm )
                                       Groundwater level [-|0]
* 01-Jan-1901 -100.0
* 31-Dec-1926 -100.0
* end table
* LboOpt = Flux (flux lower boundary condition)
                FlvLiqLboAvg (m.a-1) Average annual lower boundary flux [-1|1]
-0.250
                              (m)
                                        Amplitude of lower-boundary flux [0|0.5]
Day of maximum flux [01-Jan|31-Dec]
0.10
                FlvLiqLboAmp
01-Oct
                DayFlvLiqLboMax
* LboOpt = Head (head lower boundary condition)
Elliptic
               OptShapeGrwLev
                                         Elliptic, Parabolic, Sinusoidal, NoDrains
              HeaDrabase
RstAqt (d)
HeaAqfAvg (m)
TrafAmp (m)
-1.1
                                        Drainage base to correct GrwLev [-100|0]
                                       Resistance of aquitard [0|1e4]
500.0
                                       Mean hydraulic head of aquifer [-10|10]
-1.4
                                        Amplitude of aquifer hydraulic head [0|10]
0.2
01-Apr
                TimHeaAqfMax
                              (d)
                                         Day with maximum head [01-Jan 31-Dec]
* LboOpt = FncGrwLev (flux boundary condition - flux is a function of groundwater level)
          CofFncGrwLev (m.d-1) Coefficient in Q(h) relationship [-1|1]
ExpFncGrwLev (m-1) Exponent in Q(h) relationship [-100|100]
-0.01
-1.4
* 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
                NumDraLev
                                         Number of drainage levels (0|5)
0
* 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 [10 1e5]
100.0
                RstInf 1
                              (d)
                                         Infiltration resistance
                                        Distance between drains or channels [1|1e6]
20.0
                DistDra_1
                              (m)
                                         Bottom of drain system [0|10]
1.5
                ZDra 1
                              (m)
                TypDra_1
                                         Type of drain system: Drain or Channel
Drain
                ZSurWat 1
                             (m)
                                         Channel water level (if TypDra_1 = Channel;
1.5
                                          otherwise dummy values)
```

* If OptDra set to 'Extended' parameters below should be specified for each drainage level: 1 SysDra_1 Drainage system 100.0 (d) Drainage resistance [10]1e5] RstDra 1 100.0 (d) RstInf 1 Infiltration resistance 20.0 DistDra_1 (m) Distance between drains or channels [1 | 1e6] 1.0 Bottom width of drain system WidthDra_1 (m) 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]] OptSrfWat Option to consider surface water system No * If OptSrfWat set to `Yes' then the following parameters should be specified: SrfWatLevWinter (m) 1.0 Winter surface water level 1.0 SrfWatLevSummer (m) Summer surface water level SrfWatSupCap 0.0 (m.d-1) Surface water supply capacity _____ * Section 5: Compound section * Description _____ * 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) end table * Example for a pesticide with two daughters, named "met1" and "met2": * Line 1: pest is transformed into metl (25%), met2 (70%) and undefined end products (5%) * Line 2: metl 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 1.00 * 0.00 0.00 met2 * end_table * Transformation rate parameters **OptDT50_pest** DT50Ref_pest (d) Option for DT50: Input or Calculate Input 50.0 Half-life time [1|1e6] Temperature at which DT50 is measured [5|30] 20.0 TemRefTra_pest (C) 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 1.00 1 0.95 2 0.74 3 4 0.33 5 0.00 б 0.00 end_table * Freundlich equilibrium sorption pH-independent OptCofFre_pest pH-dependent, pH-independent, CofFre Reference conc. in liquid phase [0.1|-] 1.0 ConLiqRef_pest (mg.L-1) 0.9 ExpFre_pest (-) Freundlich sorption exponent [0.1 | 1.3] * If pH-independent (use the coefficient for sorption on organic matter): KomEql_pest (L.kg-1) Coef. eql. sorption on org. matter [0|1e9] 70.00

* 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](-) pHCorrection 0.0 pH correction [-2|1] (-) * If CofFre (specify the depth dependence and the coefficient for equilibrium sorption): KSorEql_pest (L.kg-1) MolEntSor_pest (kJ.mol-1) 1.0 Coef. for equilibrium sorption [0 | 1e9] 0.0 **TemRefSor_pest** (C) 20.0 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 6 0.00 end_table * End If * Gas/liquid partitioning PreVapRef_pest (Pa) 0.0 Saturated vapour pressure [0|2e5] TemRefVap_pest (C) 20.0 .. measured at [0|40] MolEntVap_pest (kJ.mol-1) Molar enthalpy of vaporisation [-200|200] 100.0 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 Coefficient for uptake by plant [0|10] 0.5 FacUpt_pest (-) * Canopy processes Lumped OptDspCrp**_pest** Lumped or Specified * If Lumped: 1.d6 DT50DspCrp**_pest** (d) Half-life at crop surface [1|1e6] * If Specified: 1.d6 DT50PenCrp**_pest** (d) Half-life due to penetration [1|1e6] 1.d6 DT50VolCrp**_pest** (d) Half-life due to volatilization [1 16] 1.d6 DT50TraCrp**_pest** (d) Half-life due to transformation [1|1e6] * End If 1.d-4 FacWasCrp**_pest** (m-1) Wash-off factor [1e-6|0.1] * Diffusion of solute in liquid and gas phases CofDifWatRef_pest (m2.d-1) Reference diff. coeff. in water [10e-5|3e-4] 4.3d-5 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 * Description *_____ _____ (m) Depth of Focus target layer [0.1|Z(N)-1]
 (a) Repeat interval of events [NoRepeat|1|2|3] 1.0 ZFoc DelTimEvt 1

* Event table:

```
* 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]
* End If
table Applications
01-Emg-01 AppSolSur 1.0
end_table
* Tillage table - can be empty
table TillageDates
end_table
*_____
* Section 7: Initial and boundary conditions of pesticide fate model
* Description
*
      _____
* Initial conditions
                                        Concentration in equilibrium domain [0]-]
* If using metabolites, ConSysEql should be specified for all metabolites
table interpolate CntSysEql (mg.kg-1)
       pest
z
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
*_____
* Section 8: Crop section
* Description
*_____
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
01-Nov-1901
             10-Aug-1902 WCEREALS1
end_table
* Crop cycle fixed or variable (calculated from temperature sum)
Fixed OptLenCrp
                                        Fixed or Variable
* If OptLenCrp = Variable:
            TemSumSta_WCEREALS1(C)Start value of temperature sum [-10|20]TemSumEmgAnt_WCEREALS1(C)Sum from emergence to anthesis [0|1e4]TemSumAntMat_WCEREALS1(C)Sum from anthesis to maturity [0|1e4]
0.0
0.0
0.0
* 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
                                                                   [0]10]
                                                      (m)
      LAI FacCrp ZRoot HeightCrp
table CrpPar_WCEREALS1
0.0
      0.0
           1.0 0.0
                          0.0
0.655 0.1
             1.0
                   0.2
                          0.0
0.755 3.8
             0.74
                  1.1
1.1
                          0.0
1.0
      3.8
            0.74
                          0.0
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_WCEREALS1
0.00
           1.00
1.00
            1.00
end_table
* Crop water use
                HLim1_WCEREALS1 (cm)
0.0
                                          Anaerobiosis point [-100|0]
-1.0
                                          Wet reduction point [-1000 0]
                HLim2_WCEREALS1 (cm)
-500.0
                HLim3U_WCEREALS1 (cm)
                                          Dry reduction point [-10000 0]
-900.0
                HLim3L_WCEREALS1 (cm)
                                          Dry reduction point [-10000 0]
-16000.0
                HLim4_WCEREALS1 (cm)
                                          Wilting point
                                                            [-16000|0]
70.0
                RstEvpCrp_WCEREALS1 (s.m-1)
                                              Min. canopy resistance [0|1000]
0.39
                CofExtDif_WCEREALS1 (-)
1.0
                CofExtDir_WCEREALS1 (-)
0.2
                ZTensioMeter_WCEREALS1 (m)
-100.0
                PreHeaIrrSta_WCEREALS1 (cm)
1.d-4
                CofIntCrp_WCEREALS1
                                    (cm)
                                             Constant in Braden eq for interception [0|1]
*_____
* Section 9: Output control
* Description
*_____
                                                       _____
* 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
           : Print years
* Years
             DateFormat
DaysFromSta
                                          Format of time column in output file
               OptDelOutFiles
No
               PrintCumulatives
Yes
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
0.1
0.2
0.3
0.4
0.5
0.75
1.0
2.0
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 2.0.9e * General variables print_GrwLev Groundwater level (m) Yes print_LAI Leaf Area Index (m2.m-2) Yes No print_ZRoot Rooting depth (m) print_FacCrpEvp No Crop factor (-) Soil cover (-) No print FraCovCrp print_AvoLiqErr Water balance error (m) No No print_StoCap Phreatic storage capacity (m3.m-2) No print_AvoLiqSol Amount of water in soil No print_ZPnd Ponding depth (m) * State variables print_Tem Soil temperature (C) Yes print_Eps No Volumic air content (m3.m-3) print_Theta Volumic soil water content (m3.m-3) Yes No print_PreHea Soil water pressure head (m) * Volumic volume rates (m3.m-3.d-1) print_VvrLiqDra Volumic volume rate of drainage Yes Yes print_VvrLiqUpt Volume flux of water uptake * Volume fluxes (m3.m-2.d-1) print_FlvLiq Volume flux of vertical soil water flow Yes Volume flux of precipitation Yes print_FlvLiqPrc print_FlvLiqIrr Volume flux of water in irrigation No Yes print_FlvLiqLbo Volume flux of water leaching from the soil system print_FlvLiqEvpIntPrc Evaporation flux of intercepted rainfall No No print_FlvLiqEvpIntIrr Evaporation flux of intercepted irrigation Yes print_FlvLiqEvpSol Volume flux of evaporation from the soil surface No print_FlvLiqEvpSolPot Idem, potential print_FlvLiqTrp Volume flux of transpiration by plant roots Yes 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 print_FlvLiqDra_3 Volume flux of drainage to level 3 No print_FlvLiqDra_4 Volume flux of drainage to level 4 No Volume flux of drainage to level 5 No print_FlvLiqDra_5 print_FlvLiqGrw Volume flux groundwater recharge No * Section II : Output from the PEARL model * Remark: All fluxes are averages over the print interval *_____ * Time step print_DelTimPrl Average time-step during the print interval (d) No * Mass balance (kg.m-2) Yes print_AmaEqlPro Areic mass in equilibrium domain of tillage layer Areic mass in equilibrium domain of profile print_AmaEqlTil Yes Areic mass in equilibrium domain of focus layer Areic mass in non-eql. domain of profile Yes print_AmaEqlFoc Yes print_AmaNeqPro Areic mass in non-eql. domain of tillage layer Yes print_AmaNeqTil Yes print_AmaNeqFoc Areic mass in non-eql. domain of focus layer Areic mass of pesticide in the system Yes print_AmaSysPro Areic mass of pesticide in the tillage layer Yes print_AmaSysTil Areic mass of pesticide in the focus layer Yes print_AmaSysFoc print_AmaAppSol Yes Areic mass applied to the soil system Areic mass of lateral discharge Yes print_AmaDraPro Areic mass of formation Yes print_AmaForPro print_AmaTraPro Areic mass of pesticide transformation Yes Yes print_AmaUptPro Areic mass of pesticide uptake Areic mass of drainage to level 1 Yes print AmaDra 1 Areic mass of drainage to level 2 Yes print_AmaDra_2 Yes print_AmaDra_3 Areic mass of drainage to level 3 Yes print_AmaDra_4 Areic mass of drainage to level 4 print_AmaDra_5 Areic mass of drainage to level 5 Yes print_AmaErrPro Areic numerical mass error Yes * Pesticide concentrations (kg.m-3) and contents (kg.kg-1) Yes print_ConLiq Concentration in liquid phase print_ConGas No Concentration in gas phase Concentration in equilibrium domain Concentration in non-equilibrium domain No print_ConSysEql print_ConSysNeq No Yes print_ConSys Concentration in the soil system Mass content at soil solid phase print_CntSorEql No

Yes	print_ConLigSatAvg	Avg. conc.in lig. phase between 1-2 m
Yes	print_ConLiqLbo	Concentration in percolate
Yes	print_ConLiqDra	Concentration in drainage water
Yes	print_ConLiqDra_1	Concentration in drainage water, system 1
Yes	print_ConLiqDra_2	Concentration in drainage water, system 2
Yes	print_ConLiqDra_3	Concentration in drainage water, system 3
Yes	print_ConLiqDra_4	Concentration in drainage water, system 4
Yes	print_ConLiqDra_5	Concentration in drainage water, system 5
* Pesticide	mass fluxes (kg.m-2.d-1)	
Yes	print_FlmLiq	Pesticide mass flux in liquid phase
No	print_FlmGas	Pesticide mass flux in gas phase
No	print_FlmSys	Total pesticide mass flux (FlmLig+FlmGas)
Yes	print_FlmLiqLbo	Accumulated mass flux at the lower boundary
No	print_FlmLiqInf	Accumulated mass flux of pesticide infiltration
Yes	print_FlmGasVol	Accumulated mass flux of pesticide volatilisation
* Canopy in	teraction	
*		
Yes	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
	arl input file	
*		